



15 PhD STUDENTS AND YOUNG RESEARCHERS CONFERENCE



BOOK OF ABSTRACTS



PHD STUDENTS AND YOUNG RESEARCHERS CONFERENCE

PROGRAM

OCTOBER 21st

15



	A101	D401
09:00	Opening remarks	
	Chair: dr. Vincentas Mindaugas Mačiulis	
	O1 Agnė Boguševičė E. meliloti pagrįstų MKE naudojimas žemės ūkio mėginių analizei	
	O2 Did not attend	
	O3 Muhammad Usman Khalid Tailoring niobium pentoxide nanoparticles via distinct chemical routes: structural characterization and antibacterial evaluation	
09:10-10:55	O4 Viktorija Reinikováitė Back to basics: Geometric surface area as the most relevant metric for graphite granule bioanodes	
	O5 Justina Stonytė Electrochemical Pathways to Archaeological Fungal Detection: Integrating B-Vitamin Derived Polymer Sensors, Stable Isotopes, and Yeast Genomics	
	O6 Mantvydas Usvaltas Affinity Evaluation of Polyclonal Human Antibodies to Antigen from a Repurposed Vaccine Using an Optical Method	
	O7 Tadas Jelinskas Jėgų spektrometrijos taikymas tiriant mikrogravitacijos poveikį audinių modeliams	
11:00-12:00	Meeting of the FTMC Director and the Head of the Doctoral School with FTMC doctoral students	
12:00-13:00	Lunch break	
	Chair: dr. Justinas Jorudas	Chair: dr. Lena Golubewa
	O8 Did not attend	O15 Ivan Halimski Optical properties of trans-stilbene in different phases: monomers, aggregates and crystallites
	O9 Mohammad Esmaeil Daraei Phase-Change Vanadium Dioxide Metamaterial Absorber with Radial Symmetry at Terahertz Frequencies	O16 Enayat Mohsenzadeh Rational Design of Molecularly Imprinted Polymer for Melamine and Cyanuric Acid Detection: A DFT Approach
13:00-14:45	O10 Maxim Moscotin Modified Edge-Gating Geometry of High-Electron-Mobility Transistors for Terahertz Detection	O17 Tripura Ganti NiZn/Ti and Au(NiZn)/Ti Anode catalysts for Borohydride Oxidation in Clean Energy Systems
	O11 Simonas Driukas THz spectroscopy of GeSn films for ultrafast optoelectronic applications	O18 Pamela Rivera Bismuth-Doped Laser-Induced Graphene Electrodes for Simultaneous Detection of Zn ²⁺ , Pb ²⁺ , and Cd ²⁺
	O12 Karolis Galvanauskas Stibidų pagrindo infraraudonosios spinduliuotės fotodetektoriai	O19 Ilya Navitski Heavy metal sensing capabilities of MXenes and potential applications in protein detection
	O13 Austėja Trečiokaitė Didelio pralaidumo erdvinė-laikinė optinė koherentinė tomografija	O20 Aswathi Raveendran Comparative study of amino acids influence on the hydrothermally synthesized CoFe ₂ O ₄ nanoparticles
	O14 Justina Žemgulytė Cilindrinės rezonansinės antenos radijo bangų energijos rinkimui	O21 Saqib Ali Au Functionalized MXene for Plasmonic Detection of Organic Molecules in Water
14:45-15:00	Break	
	Chair: dr. Tomas Daugalas	Chair: dr. Nadežda Traškina
	O22 Pavel Piatrou Magnetic field dynamics during magnetic pulse forming and crimping	O29 Germantė Paulikaitė Surface-Modified MXenes as Promising Adsorbents for Organic Pollutant Elimination
	O23 Darius Antonovič Development and Characterization of CoFe/Cu-based Spin-Valves	O30 Gytautė Sirgėdaitė Bimetalinės nanostruktūros sustiprinto Ramano sklaidos tyrimams
	O24 Ifra Bibi Laser Induced Single Photon Emitters in Hexagonal Boron Nitride for Quantum Key Distribution	O31 Virginija Ulevičienė Azotų ir metalais legiruotos biomasinės anglies katalizatorių (AWC-Co-N, AWC-Cu-N) sintezė ir jų taikymas hidrazino oksidacijai
15:00-16:45	O25 Seda Türkcan Carrier Dynamics in n- and p-type InGaN Layers	O32 Huma Amber Cobalt-Based Electrocatalysts: A Pathway Toward Cost-Effective and High-Performance Water Splitting
	O26 Muhammad Adnan Saeed Directly Grown Graphene on Annealed and Non-annealed SiO ₂ Films of Different Thicknesses	O33 Gitana Valeckytė Nikelio-kobalto dangų cheminis nusodinimas ir taikymas vandenilio generavimui
	O27 Aivaras Špokas Extending Bismide Emitter Applications from Medicine to Telecommunication	O34 Tomas Paškevičius Development of Electron Deficient Phosphine Ligands for Palladium(II) Catalysed Fluorination of Arenes
	O28 Deividas Vainauskas SbSeI dangų nusodinimo optimizavimas terminio garinimo metodu	
17:00-18:30	Success is a Habit or How to Awaken Your Motivation: interactive lecture for PhD students by Rima Vanagė	
18:30	FTMC PhD Student Community Gathering	

PHD STUDENTS AND YOUNG RESEARCHERS CONFERENCE

15



PROGRAM

OCTOBER 22nd

	A101	D401
	Chair: dr. Ada Steponavičiūtė	Chair: dr. Laurynas Bučinskas
	O35 Julius Lukošius Photodarkening in BGSe and BGGSe	O45 Karolis Daugevičius Star cluster size evolution in the Andromeda galaxy
	O36 Julianija Nikitina Submicron Periodic Structures in Metal Oxide Thin Film via Laser Ablation and Thermal Oxidation	O46 Agnė Minderytė City-produced and transported black carbon: synergy of in-situ optical measurements and modeling
	O37 Darija Astrauskytė Nanostruktūrizuotų dangų stabilizavimas naudojant atominių sluoksnių nusodinimo technologiją	O47 Durre Nayab Habib Tracing Photochemical Aging in Biomass Burning Aerosols Using Carbon Isotopes
	O38 Vita Petrikaitė Lazerinis nanodalelių generavimas iš Ti-Au plonų dangų plazmoninių spalvų analizei	O48 Viachaslau Alifirenka Source apportionment of aerosol particles by positive matrix factorization in urban background environment (Vilnius, Lithuania)
9:00-11:30	O39 Kernius Vilkevičius Hibridinės sidabro-aukso bimetalinės nanogardelės, skirtos plazmonų rezonanso sensorikai	O49 Sonata Pleskytė Impact of the physical properties of LDPE mulch films on photocatalytic degradation efficiency under UV irradiation
	O40 Rodrigas Liudvinavičius Aukso ir sidabro mikrogumbelių gardelės žadinančios plazmonų rezonansą	O50 Kristina Mikalauskiene Development of the Non-Destructive Method for the Determining Surface Contamination in Radioactive Waste
	O41 Karolis Stravinskas Mechanical and Thermal Property Optimization of SiC-Reinforced AlSi10Mg Composites via DMLS	O51 Mahrosh Javed Development of modified graphene oxide nanocomposite for the removal of nanoplastics from fresh water
	O42 Dainius Balkauskas Design and Investigation of SSAIL Transparent Electrodes on Glass for Electrochromic Applications	O52 Tayyab Tahir Development of Magnetic Buckwheat Hull-Fe ₃ O ₄ Nanocomposite for Biosorption of Pb(II), Cd(II), and Cr(III) from Mixed Heavy Metal Wastewater
	O43 Ioanna-Angeliki Petsi Two-Photon Polymerization of Low-Density Micro-Targets and Assembly into Rigid Holders for Inertial Confinement Fusion Studies	O53 Gediminas Skarbalius CFD Modeling and Optimization of Forced-Air Cooling in Indoor LiFePO ₄ Battery Energy Storage Cabinets
	O44 Lukas Šalavėjus Design of Wide Input Voltage Range DC-DC Converter Integrated Circuit for Automotive Applications	
12:00-13:00	Lunch break	
13:00-15:00	Poster Session (near A101)	

PHD STUDENTS AND YOUNG RESEARCHERS CONFERENCE

15



POSTERS

near A101, 13:00-15:00

	near A101, 13:00-15:00
P1	Did not attend
P2	Bilal Islam Additive Manufacturing Approach for the Development of Piezoelectric Polymer–Ceramic Composites
P3	Gabrielė Rankelytė Impact of the Protein Environment on the Excited States of the Pigments in Photosynthetic Complexes
P4	Greta Kasputė Molecularly imprinted polymers as selective recognition elements for geraniol detection
P5	Paulius Baronas Systematic Study of Sulfuric Acid Anodization Parameters for Satellite Grade Aluminum Alloys
P6	Kamilė Kasperavičiūtė Improving membrane coating approaches to promote cell adhesion in two-channel microphysiological systems
P7	Felix Lücke Development of a Biocompatible Polymer-Based Drug Delivery System
P8	Raiane Rodrigues da Silva Pea albumin modification by Pulsed Electric Field (PEF)
P9	Kamila Turuta Synthesis of photoelectrochemically active g-C ₃ N ₄ layers
P10	Marijus Mozdeikis Difrakcinių gardelių periodo ir lazerio impulso energijos tyrimas aukštos kokybės plazmoniniams rezonansams ant ITO padėklų taikant tiesioginį lazerinį rašymą
P11	Barbora Škėlaitė Terahertz Spectroscopy of Semiconductor Metasurfaces in GaAs Based Structures
P12	Patricija Ivanauskaitė Methanol Spectroscopy at 257 GHz Employing CMOS-Based Optopair
P13	Justina Vaičaitytė Kvantinio dimero modeliavimas sukabintais klasikiniais harmoniniais osciliatoriais
P14	Paulius Kizevičius Plokščiųjų THz optikos elementų palyginimas skaitmeniniame vaizdinimo eksperimente
P15	Jorūnas Dobilas Monte Carlo Study of the Self-assembly of INDO ₄ Molecules on Ag Surfaces
P16	Justas Žuvelis Impact of AlGaAs Barrier Composition and Profile on the Emission of InGaAs Quantum Wells
P17	Giedrius Puidokas Search for High Triplet Energy Hosts for Stable Blue TADF OLEDs
P18	Mehri Davtalab Investigating the effects of urban structure on urban heat island using machine learning
P19	Aistė Štaupienė Improved Emission Properties of GaAsBi QWs due AlGaAs Graded Barrier Design and Thermal Annealing
P20	Lukas Stacevičius Integration of Digital Terahertz Holography and Light Scattering Modeling in Granular Material Analysis
P21	Miglė Stančiauskaitė Label-Free Immunosensing of AmpC Beta-Lactamase Using Combined SE/QCM-D Method with Subclass-Dependent IgG Capture Layers
P22	Patricija Strumilaitė GaAsBi/(Al,Ga)As kvantinių duobių atkaitinimo greito atkaitinimo krosnyje tyrimas
P23	Karolis Mundrys Fotonių elementų taikymas vieno pikselio THz vaizdinime
P24	Gabriel Slabošev Electrochemical Sensor for Salicylic Acid Based on a Molecularly Imprinted Polypyrrole
P25	Andžej Borel RF galios stiprintuvų elgsenos modeliavimas naudojant interpoliuotus atminties polinomus

PHD STUDENTS AND YOUNG RESEARCHERS CONFERENCE

15



POSTERS

near A101, 13:00-15:00

P26	Artem Yerniazov Nanofilm conductive polymer MIP platform for detection of BSA
P27	Danielius Ragoža Optimization of Exposure Parameters for SLA-Fabricated SiO ₂ Nanoceramic Composites
P28	Dainius Ratkus Femtosecond laser ablation and polishing of silicon carbide wafers by bursts
P29	Brigita Žakevičiūtė Vienfazio pulsuojančio srauto dinamikos ir struktūros mikrokanaaluose tyrimas
P30	Gintarė Ruginytė Design and Application of MXene–Noble Metal Nanostructure Composites for Colourimetric Water Quality Testing
P31	Deividas Rūškys Formation of H, C, Si, La Ion targets to use in the Negative Cs-sputtering Ion source Hiconex
P32	Evita Spalinskaitė Plasmon–exciton polaritonic emission lifetime dynamics under strong coupling
P33	Jonas Paukštys Electron-deficient phosphine ligands for palladium catalysed C–N cross-coupling reactions
P34	Edgard Aleinikov Comprehensive Literature Review of Thermal and Electrical Challenges in Electro-Optic Pulse Drivers
P35	Mantas Mackelis Leidenfrosto garo plėvelės poveikio karšto kūno šilumos perdavimui skaitinis modeliavimas
P36	Dovilė Vasiliauskaitė Investigation of New Electron-Transporting Materials in Perovskite Solar Cells Using the Kinetic Photoconductivity Method
P37	Rugilė Pečiulytė Priverstinės Briliueno sklaidos lazerio impulsų spaustuvus naudojant HT-230 skystį
P38	Robertas Virkėtis YAG:Ce 3D mikrostruktūrų gamyba naudojant dvifotonę polimerizaciją ir kalcinaciją
P39	Jelizaveta Fedotova Investigation of Spectroscopic Properties of Free-Base Tetraphenylporphyrin and Hexagonal Boron Nitride Van Der Waals Complex
P40	Noor ul Ain Ahmed Charge Carrier Dynamics at the Perovskite/Graphene–MoO ₃ Interface
P41	Titas Tamošauskas Elektrochrominių sluoksnių ir skaidrių vario takelių elektrodų spektrinis tyrimas
P42	Samanta Gelumbickytė Microfluidic Preparation of Chitosan Nanoparticles for Drug Delivery
P43	Dmytro Shyshkin Enhanced Performance of Gold Nanoparticles Modified Nickel-Iron for Sodium Borohydride Oxidation
P44	Daumantas Sriubas Formation of channels in soda-lime glass using a laser ablation and chemical etching through a thin chromium layer mask
P45	Ugnė Šilingaitė Terahercinių vaizdų raiškos gerinimas naudojant neuroninius tinklus
P46	Milda Valytė Ar kosmologiniai modeliai atkuria stebimas galaktines tėkmes?
P47	Eimantas Dermauskas Fazės pokyčio priklausomybė nuo geometrijos formuojant daugiasluoksnes modifikacijas lydytame kvarce femtosekundiniu lazeriu
P48	Paulius Rindzevičius Polikristalinių deimantinių darinių su metalinėmis nanostruktūromis KARS tyrimas/CARS study of polycrystalline diamond structures with metal nanostructures
P49	Aidas Mikalauskas Bismuto koncentracijos įtaka GaAs _{1-x} Bi _x optinėms savybėms
P50	Did not attend
P51	Adomas Strazdas Humidity-Induced Stress Variations in Nanostructured GLAD Coatings for High-LIDT Optical Mirrors

E. meliloti pagrįstų MKE naudojimas žemės ūkio mėginių analizei

Agnė Boguševičė¹, Tomas Mockaitis¹, Inga Morkvėnaitė-Vilkončienė¹

1. Fizinių ir technologijos mokslų centras, Nanotechnologijų skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: agne.bogusevice@ftmc.lt

Pasauliui kovojant su klimato kaita, mikrobiniai kuro elementai (MKE) siūlo perspektyvią alternatyvą išskatiniam kurui. Tai bioelektrocheminės sistemos, kuriose mikroorganizmai, anaerobiškai skaidydami organines medžiagas, cheminę energiją paverčia elektra [1]. Ši technologija yra dvejopai naudinga, tai ne tik gamina tvarią energiją, bet ir leidžia iš aplinkos pašalinti organinius teršalus, panaudojant juos kaip kurą [2]. Nors deguonis dažniausiai naudojamas kaip elektronų akceptorius, siekiant didesnio efektyvumo nuolat ieškoma naujų alternatyvų, todėl MKE yra itin patraukli atsinaujinančios energetikos sritis [3].

Ensifer meliloti (*E. meliloti*) yra dirvožemio bakterija, atliekanti esminį vaidmenį žemės ūkyje – azoto fiksaciją. Ji sudaro simbiotinį ryšį su ankštiniais augalais, reaguodama į jų išskiriamus cheminius signalus [4]. Prisitraukusios prie šaknų, bakterijos skatina mazgelių formavimąsi, kuriuose jos virsta specializuotomis struktūromis – bakteroidais. Šiuose mazgeliuose, kur augalo gaminamas leghemoglobinas sukuria žemos deguonies koncentracijos aplinką, o *E. meliloti* atmosferos azotą paverčia augalams prieinamu amoniaku, kurį jie gali įsisavinti. Tai svarbus biologinio tręšimo mechanizmas, mažinantis cheminių trąšų poreikį.

Tyrimo tikslas *E. meliloti* panaudojimas mikrobiniuose kuro elementuose žemės ūkio mėginių analizei. Našumui gerinti taikomi chinonų redokso mediatoriai, kurie palengvina elektronų perdavimą iš bakterijų į elektrodą.

Literatūra

1. Ramanavicius, S.; Ramanavicius, A. Charge Transfer and Biocompatibility Aspects in Conducting Polymer-Based Enzymatic Biosensors and Biofuel Cells. *Nanomaterials* 2021, 11, 1–22. doi.org/10.3390/nano11020371
2. Reinikovaite, V.; Zukauskas, S.; Zalneravicius, R.; Ratautaite, V.; Ramanavicius, S.; Bucinskas, V.; Vilkiene, M.; Ramanavicius, A.; Samukaite-Bubniene, U. Assessment of Rhizobium anhuiense Bacteria as a Potential Biocatalyst for Microbial Biofuel Cell Design. *Biosensors* 2023, 13, 66. doi.org/10.3390/bios13010066
3. Rozene, J.; Morkvenaite-Vilkonciene, I.; Bruzaite, I.; Dziedzickis, A.; Ramanavicius, A. Yeast-based microbial biofuel cell mediated by 9,10-phenanthrenequinone. *Electrochim Acta* 2021, 373 [doi: 10.1016/j.electacta.2021.137918](https://doi.org/10.1016/j.electacta.2021.137918)
4. Bendinskaite, S.; Bruzaite, I.; Rožėnė, J.; Mockaitis, T.; Morkvenaite-Vilkonciene, I.; Ramanaviciene, A.; Zinovicius, A., & Ramanavicius, A. (2024). Microbial Fuel Cell Based on Ensifer meliloti. *Journal of the Electrochemical Society*, 171(10) doi.org/10.1149/1945-7111/ad8037

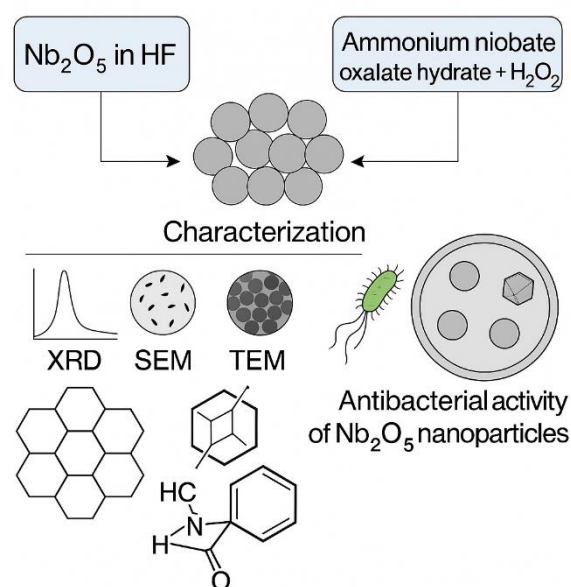
O2 Did not attend.

Tailoring niobium pentoxide nanoparticles via distinct chemical routes: structural characterization and antibacterial evaluation

Muhammad Usman Khalid¹, Vidas Pakstas², Arunas Stirke¹, Monika Kirsnytė¹, Wanessa De Melo¹

1. Department of Functional Materials and Electronics, State Research Institute Centre for Physical Sciences and Technology (FTMC), 10257 Vilnius, Lithuania
2. Department of Characterization of Materials Structure, State Research Institute Centre for Physical Sciences and Technology (FTMC), 10257 Vilnius, Lithuania

Niobium pentoxide (Nb_2O_5) nanoparticles are promising for biomedical applications due to their adjustable physicochemical features (1,2). Nb_2O_5 nanoparticles were synthesised using two chemical routes: (i) direct dissolution of Nb_2O_5 in hydrofluoric acid (HF), and (ii) reaction of ammonium niobate(V) oxalate hydrate with hydrogen peroxide (H_2O_2). X-ray diffraction, electron microscopy, and dynamic light scattering revealed route-dependent changes in crystallinity, size, and dispersion. H_2O_2 -derived nanoparticles (12 g/L) showed the maximum efficiency against *Escherichia coli* due to their ultra-small crystallites (~ 4.5 nm), monodispersity ($\text{PDI} = 0.118$), and superior colloidal stability. The 5 g/L HF sample demonstrated high antibacterial activity, likely due to increased particle concentration despite a broader size dispersion. Mechanistic studies indicated that the bactericidal effects connected with increased reactive oxygen species. The 5 g/L HF sample demonstrated high antibacterial activity, possibly due to enhanced particle concentration despite its broader size dispersion. Mechanistic investigations found that bactericidal effects were associated with increased reactive oxygen species (ROS) formation, especially in H_2O_2 -synthesized nanoparticles with oxygen-defect architectures. ICP-MS indicated minimal but detectable Nb ion release, indicating that ROS generation, not ion leaching, was the primary antibacterial mechanism. Nb_2O_5 nanoparticles' antibacterial activity depends on their synthesis technique and precursor concentration, indicating their potential for biological uses.



References

1. Rani, Rozina Abdul, et al. "Thin films and nanostructures of niobium pentoxide: fundamental properties, synthesis methods and applications." *Journal of Materials Chemistry A* 2.38 (2014): 15683-15703.
2. Raba, Angela M., Jorge Bautista-Ruiz, and Miryam R. Joya. "Synthesis and structural properties of niobium pentoxide powders: a comparative study of the growth process." *Materials Research* 19.6 (2016): 1381-1387.

Back to basics: Geometric surface area as the most relevant metric for graphite granule bioanodes

Viktorija Reinikovaite^{1,2}, Matthias Schmidt², Falk Harnisch², Arūnas Stirke¹, and Benjamin Korth²

1. Center for Physical Sciences and Technology, Department of Functional Materials and Electronics
Saulėtekio av. 3, LT-10257 Vilnius, email: viktorija.reinikovaite@ftmc.lt
2. Helmholtz Center for Environmental Research GmbH – UFZ, Department of Microbial Biotechnology
Permoser Str. 15, 04318 Leipzig, Germany

Graphite granules (GG) are commonly used as three-dimensional electrode material in microbial electrochemical technologies (METs) due to their cost-effectiveness and biocompatibility, offering a high surface-to-volume ratio in fixed-bed electrode reactors¹. While GG have been increasingly studied in MET over the past decade for applications such as wastewater treatment and electrobioremediation, defining the *relevant* surface area for electroactive biofilms is not trivial². Standard Brunauer-Emmett-Teller (BET) analysis measures the total surface area, including micropores inaccessible to bacteria, leading to a substantial overestimation of the electroactive area and inaccurate current density calculations. In contrast, calculating the surface area assuming ideal spheres likely underestimates the accessible area. This discrepancy leads to significant inaccuracies in normalizing electrochemical performance metrics such as current density, hindering reliable comparisons with literature data³, lab-scale experiments using monolithic electrodes and realistic performance assessments of fixed bed electrode reactors.

To resolve this, we systematically compared four surface area determination methods for individual GG, which probe different scales of surface topography (Fig 1): i) BET analysis, measuring the total surface area including microporosity; ii) underpotential copper deposition, an electrochemical method sensitive to the atomically rough surface and pores accessible to the electrolyte; iii) cyclic voltammetry with a ferro/ferricyanide redox probe, another electrochemical method assessing the area accessible to dissolved redox species; and iv) a geometric approximation combining profilometry with water displacement to overcome the limitations of either technique alone and provide a robust estimate of the macroscopic surface contour. The accuracy of each method was evaluated by cultivating *Geobacter sulfurreducens* pure culture biofilms on individual GG and on smooth graphite plates, and then calculating the resulting current density based on each area value.

The determined mass-specific surface area varied considerably between $0.8 \pm 0.2 \text{ m}^2 \text{ g}^{-1}$ (BET analysis) and $0.0015 \pm 0.0004 \text{ m}^2 \text{ g}^{-1}$ (geometric approximation combined with profilometry). When these values were used to normalize the current production of mature biofilms, the geometric approximation yielded current densities that were consistent and comparable to those obtained from well-defined flat graphite plates³. In contrast, the use of BET area resulted in a dramatic, orders-of-magnitude underestimation of performance. Helium ion microscopy of *G. sulfurreducens* biofilms of different maturity states provided direct visual confirmation, showing that the microorganisms

colonized only the outer GG surface, avoiding pores with open diameters of $\sim 10 \mu\text{m}$. This observation confirms that the accessible electrode area for electroactive biofilms is defined by the granule's macroscopic geometry and surface roughness, not its microscopic porosity.

These findings revealed that for biofilm electrodes, the relevant surface area is defined by microbial accessibility, not total porosity. A geometric approximation supported by profilometry provides the most reliable metric for current density normalization, enabling accurate performance assessment and comparison with monolithic electrodes.

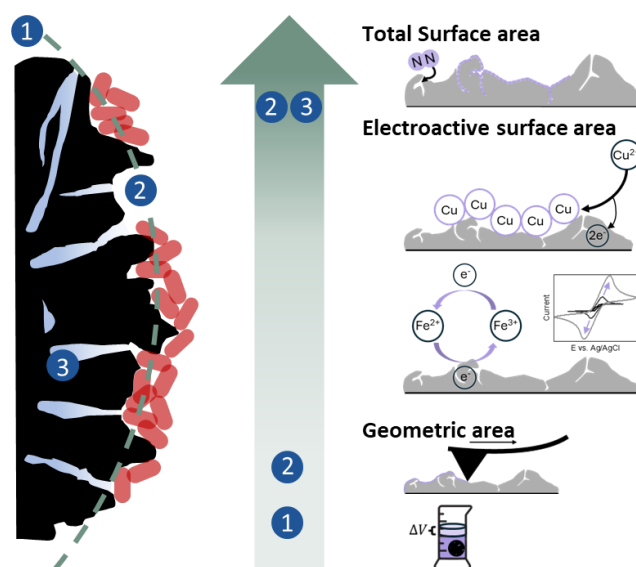


Fig 1. Illustration of complex GG surface structure and possible definition of surface area: 1 Geometric area (profilometry with water displacement). 2 ECSA via soluble redox probes and underpotential deposition. 3 total surface area based on BET analysis.

References

1. Rodrigo Quejigo, J.; Tejedor-Sanz, S.; Esteve-Núñez, A.; Harnisch, F. Bed Electrodes in Microbial Electrochemistry: Setup, Operation and Characterization. *ChemTexts* 2019, 5 (1), 4.
2. Caizán-Juanarena, L.; Sleutels, T.; Borsje, C.; Ter Heijne, A. Considerations for Application of Granular Activated Carbon as Capacitive Bioanode in Bioelectrochemical Systems. *Renew. Energy* 2020, 157, 782–792.
3. Rotaru, A.-E.; Woodard, T. L.; Nevin, K. P.; Lovley, D. R. Link between Capacity for Current Production and Syntrophic Growth in *Geobacter* Species. *Front. Microbiol.* 2015, 6.

Electrochemical Pathways to Archaeological Fungal Detection: Integrating B-Vitamin Derived Polymer Sensors, Stable Isotopes, and Yeast Genomics

Justina Stonytė¹, Paulina Morkytė¹, Aistė Tuzinaitė², Giedrė Keen Motuzaitė-Matuzevičiūtė³,
Rasa Pauliukaitė¹

1. Center for Physical Sciences and Technology, Department of Nanoengineering
Savanorių av. 231, LT-02300 Vilnius
2. Center for Physical Sciences and Technology, Department of Nuclear Research
Saulėtekio av. 7, LT-10257 Vilnius
3. Vilnius University, Faculty of History, Department of Archeology
University st. 7, LT-01513 Vilnius Email: justina.stonyte@ftmc.lt

Fungi have played multifaceted roles in human history as food, medicine, and psychoactive agents, yet their traces are poorly represented in archaeology due to limited preservation [1]. We explore an interdisciplinary framework that integrates electrochemical sensors, stable isotope analysis, and fungal genomics to reconstruct fungal use and presence in Lithuanian archaeological and cultural contexts.

The central innovation lies in the development of a B-vitamin-based electrochemical biosensor designed to detect fungal traces present in all fungi. Electrochemical sensors are particularly well-suited to fungal studies: they combine nanomolar sensitivity, selectivity, and low-resource consumption, making them especially valuable for archaeological applications where destructive methods that are usually used are impractical.

In this work, electrochemical investigations were performed with B-vitamin monomers (thiamine, riboflavin, pyridoxal) and an amino acid L-lysine. Vitamin monomers were electropolymerized directly onto electrode surfaces through cyclic voltammetry (CV), forming thin films whose properties were tuned by the number of cycles, electrolyte composition, and solution pH. The resulting polymer coatings were evaluated using CV and differential pulse voltammetry (DPV). Results showed that they can be electropolymerized into stable conductive films, they demonstrated sensitivity to biologically relevant analytes, laying the groundwork for fungal trace specific biosensors.

Parallel isotope studies established baseline $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ values for common Lithuanian mushrooms, supporting their potential as dietary markers in archaeological interpretation.

Complementing this, yeast strains collected from traditional Lithuanian brewers were isolated and characterized, revealing diverse fermentative taxa. Together, these pillars demonstrate how electrochemical sensor design is strengthened by biological baselines from isotope and genomic data, and vice versa, creating a feedback loop of these methods.

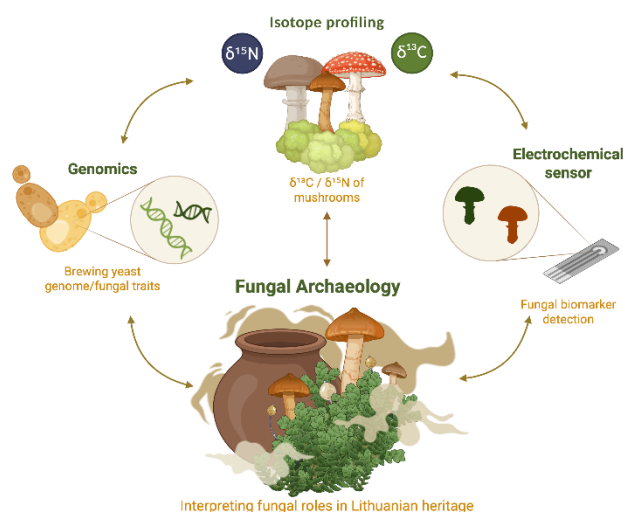


Figure 1. Schematic framework of the research electrochemical biosensor development, stable isotope profiling, and yeast genomics connect to inform fungal archaeology.

References

1. H. J. O'Regan, A. L. Lamb, and D. M. Wilkinson, 'The missing mushrooms: Searching for fungi in ancient human dietary analysis', *J. Archaeol. Sci.*, vol. 75, pp. 139–143, Nov. 2016, doi: 10.1016/j.jas.2016.09.009.

AFFINITY EVALUATION OF POLYCLONAL HUMAN ANTIBODIES TO ANTIGEN FROM A REPURPOSED VACCINE USING AN OPTICAL METHOD

Mantvydas Usvaltas¹, Vincentas Mačiulis¹, Asta Lučiūnaitė², Silvija Jučiutė^{1,4}, Almira Ramanavičienė⁴, Ieva Plikusienė^{1,3}

1. Center for Physical Sciences and Technology, Department of Nanotechnology
Saulėtekio av. 3, LT-10257 Vilnius, email: mantvydas.usvaltas@ftmc.lt
2. Institute of Biotechnology, Life Sciences Center, Vilnius University, Saulėtekio ave. 7, LT-10257 Vilnius
3. Pharmacy and Pharmacology Center, Faculty of Medicine, Vilnius University, Čiurlionio str. 21, Vilnius, Lithuania
4. NanoTechnas - Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko Str. 24, 03225, Vilnius, Lithuania

With the global rise in pharmaceutical production and consumption there was also an increase in pharmaceutical waste which can lead to significant risk to public health and the environment. Recent events involving huge vaccine production and waste, most notably the rapid development, production and distribution of vaccines against the SARS-CoV-2 virus has left a huge amount of excess unused vaccines which have by now expired [1]. Although expired vaccines are no longer suitable for their intended purpose, they may still be repurposed for applications such as biosensing, since they often retain intact antigens [2]. Biosensors developed from expired COVID-19 vaccines can be used to assess whether an individual possesses sufficient immunity against SARS-CoV-2.

Development of biosensors can be performed by applying real-time, label-free, and sensitive methods. In this work, we applied spectroscopic ellipsometry as one such method. It is a highly sensitive and non-destructive technique that measures two ellipsometric parameters: Ψ , the light wave amplitude, and Δ , the light wave phase shift. By performing the measurement in the total internal reflection ellipsometry (TIRE) mode, we can observe surface plasmon resonance, which provides high sensitivity for detecting small-molecule interactions. From the measured changes in Ψ and Δ over time, we can calculate the binding kinetics and thermodynamics of polyclonal antibody interactions with virus-like particles from repurposed COVID-19 vaccines [3].

In this work, different SARS-CoV-2 antigens—including virus-like particles derived from expired vaccines, the SARS-CoV-2 spike protein, and the SARS-CoV-2 Omicron spike protein—were covalently immobilized, and the affinities of polyclonal human antibodies in diluted sera were compared. The sera were obtained from four volunteers: one previously diagnosed with COVID-19, two vaccinated with the Comirnaty vaccine, and one vaccinated with the Vaxzevria vaccine. Using the TIRE method, we measured real-time interaction kinetics and evaluated the binding affinities of polyclonal antibodies in diluted human sera, demonstrating that virus-like particles from expired vaccines can be successfully immobilized on the functionalized 11-MUA gold biosensor surface and that polyclonal antibodies bind to them with high affinity.

References

1. J. V. Lazarus, S.S. Abdool Karim, L. Van Selm, J. Doran, C. Batista, Y. Ben Amor, M. Hellard, B. Kim, C.J. Kopka, P. Yadav, COVID-19 vaccine wastage in the midst of vaccine inequity: causes, types and practical steps, *BMJ Glob Health* 7 (2022) 17. <https://doi.org/10.1136/BMJGH-2022-009010>.
2. W.A. Prates-Syed, L.C.S. Chaves, K.P. Crema, L. Vuitika, A. Lira, N. Côrtes, V. Kersten, F.E.G. Guimarães, M. Sadraeián, F.L. Barroso da Silva, O. Cabral-Marques, J.A.M. Barbutto, M. Russo, N.O.S. Câmara, G. Cabral-Miranda, VLP-Based COVID-19 Vaccines: An Adaptable Technology against the Threat of New Variants, *Vaccines* 2021, Vol. 9, Page 1409 9 (2021) 1409. <https://doi.org/10.3390/VACCINES9121409>.
3. I. Baleviciute, Z. Balevicius, A. Makaraviciute, A. Ramanaviciene, A. Ramanavicius, Study of antibody/antigen binding kinetics by total internal reflection ellipsometry, *Biosens Bioelectron* 39 (2013) 170–176. <https://doi.org/10.1016/J.BIOS.2012.07.017>.

JĖGŲ SPEKTROMETRIJOS TAIKYMAS TIRIANT MIKROGRAVITACIJOS POVEIKĮ AUDINIŲ MODELiams

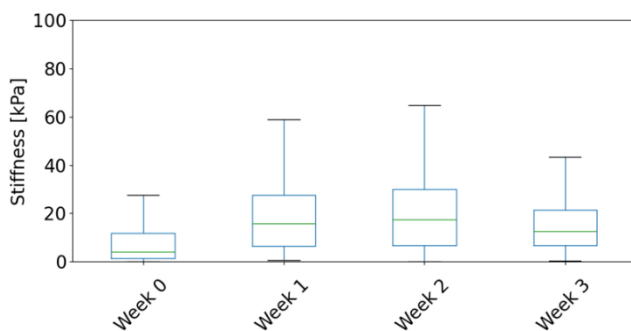
Tadas Jelinskas¹, Artūras Ulčinas¹

1. Fizinių ir technologijos mokslų centras, Nanoinžinerijos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: tadas.jelinskas@ftmc.lt

Vienas iš unikaliausių potyrių kosmoso ekspedicijų metu yra mikrogravitacija. Tokiomis sąlygomis dingsta apkrova kūnui ir astronautai gali tiesiog kabėti ore, tačiau prie mikrogravitacijos žmogaus organizmas nėra prisitaikęs. Ilgas buvimas mikrogravitacijoje sukelia eilę sutrikimų: vyksta kaulų demineralizacija, atsiranda kremzlės pažeidimai, raumenų atrofija, ir t.t. [1]. Išsiaiškinus mikrogravitacijos poveikio mechanizmus bus galima kurti tikslines priešpriešmones ilgalaikėms kosminėms misijoms.

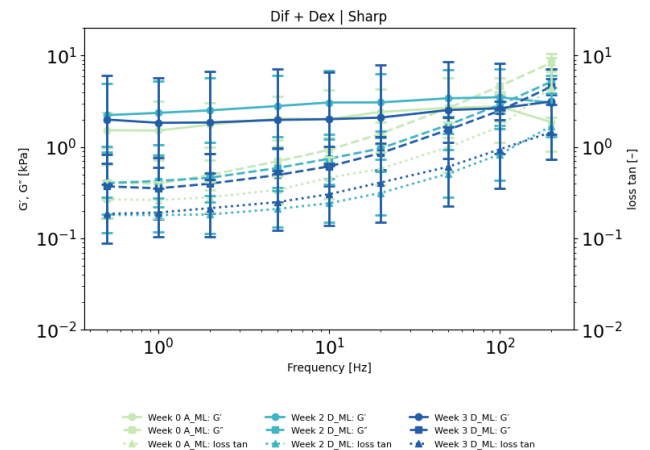
Atominių jėgų mikroskopas (AJM) yra vienas iš pagrindinių įrankių, naudojamų mechaninių savybių matavimams, galintis išmatuoti įvairius medžiagų ar ląstelių mechaninius parametrus mikro ir nanoskalėje. Sąnario kremzlės struktūra mechaniniu požiūriu yra gan sudėtinga, jos standumas makro skalėje gali kisti tarp 0,1 – 2 MPa, mikro skalėje 40 – 70 kPa [2], o pačių chondrocitų standumas siekia vos kelis kPa. AJM, dėka didelio jautrumo, plataus matavimo diapazono ir aukštos erdvinės skyros, yra tinkamas įrankis sekti mikrogravitacijos sąlygotus kremzlės audinio pakitimus atskirų ląstelių lygmeniu. Mechaninių parametrų pokyčiai normalios ir simuliuotos mikrogravitacijos sąlygomis, tikėtina, suteiks įžvalgų apie tai, kokia yra ląstelių ir besiformuojančių audinių reakcija į tokias ekstremalias sąlygas.

Norint tiksliai įvertinti kremzlės mikromechaninius parametrus pirmiausia buvo atlikti AJM matavimo protokolo optimizavimo darbai naudojant 0,1-100 kPa PAAm hidrogelių etaloninius bandinius, kurie parodė naudojamo matavimo protokolo tinkamumą. Žmogaus riebalinio audinio kamieninių ląstelių (hAdSC) diferenciacijos į chondrocitus metu atlikti pirminiai mechaninių parametrų matavimai parodė reikšmingus ląstelių standumo pokyčius lyginant su hAdSC prieš diferenciaciją ir hAdSC kontroline grupe.



pav. 1 hAdSC Jungo modulis chondrogenezės eigoje.

Matavimai buvo atliekami AJM kvazistatiniu (pav. 1) ir dinamiu režimu (pav. 2). Kvazistatiniu režimu buvo matuojamos jėgų-atstumo kreivės, iš kurių buvo apskaičiuotas ląstelių Jungo modulis. Matavimai dinamiu režimu buvo naudojami nustatant ląstelių viskoelastines savybes.



pav. 2 hAdSC viskoelastinės savybės chondrogenezės eigoje

Šie pirminiai matavimai patvirtina sukurto protokolo tinkamumą tirti ląstelių mechaninį fenotipą skirtinguose diferenciacijos etapuose, ir sudaro sąlygas įvertinti besiformuojančių audinių mechaninių savybių pokyčius įvairių aplinkos poveikių metu.

Reikšminiai žodžiai: mechanobiologija, mikrogravitacija, AJM, hAdSC, kremzlė.

Literatūra

1. Q. Zhang, M. Zhang, N. Meng, X. Wei, and W. Chen, 'Mechanobiology of the articular chondrocyte', in Bone Cell Biomechanics, Mechanobiology and Bone Diseases, Elsevier, 2023, pp. 249–287. doi: 10.1016/B978-0-323-96123-3.00016-6.
2. B. Ganse, M. Cucchiari, and H. Madry, 'Joint Cartilage in Long-Duration Spaceflight', Jun. 01, 2022, MDPI. doi: 10.3390/biomedicines10061356.
3. W. Xu, J. Zhu, J. Hu, and L. Xiao, 'Engineering the biomechanical microenvironment of chondrocytes towards articular cartilage tissue engineering', Nov. 15, 2022, Elsevier Inc. doi: 10.1016/j.lfs.2022.121043.

O8 Did not attend.

Phase-Change Vanadium Dioxide Metamaterial Absorber with Radial Symmetry at Terahertz Frequencies

Mohammad Esmaeil Daraei¹, Mehdi Abedi-Varaki², and Ignas Nevinskas¹

1. Department of Optoelectronics, Center for Physical Sciences and Technology, Saulėtekio av. 3, LT-10257 Vilnius, Lithuania.

2. Department of Laser Technologies, Center for Physical Sciences and Technology, Savanoriu av. 231, LT-02300 Vilnius, Lithuania. email: esmaeil.daraei@ftmc.lt

Recent progress in nanophotonics has significantly advanced the capability to manipulate light at scales smaller than the diffraction limit, giving rise to a wide range of emerging technologies. Despite these advances, most optical devices are designed with fixed optical properties and their behavior cannot be changed or tuned after fabrication. So, the presence of phase-change materials (PCMs) enables active modulation of optical responses by exploiting their controllable phase transitions. VO₂ is one of the most extensively studied PCMs owing to its ultrafast and reversible semiconductor-to-metal transition accompanied by a structural phase transition. In VO₂, two mechanisms Mott and Peierls [1] act cooperatively, resulting in an abrupt insulator–metal transition in which the carrier concentration increases by nearly four orders of magnitude. VO₂ is very functional in terahertz (THz) frequency ranges. THz radiation occupies the spectral region bridging the gap between microwave and infrared frequencies. The development of practical THz applications is hindered by the limited availability of high-performance functional devices, due to the lack of intrinsic materials with efficient THz wave interactions. This challenge has been addressed through the development of metamaterials, artificially designed composites characterized by periodically arranged subwavelength resonant structures. This research focuses on a numerical study of the optical behavior of a radially symmetric metamaterial absorber (MMA), consisting of alternating triangular wedges, trapezoids and semi partial rings segments made of VO₂ PCM in THz frequency ranges. This compound geometry supports multiple localized plasmonic modes characterized by strong spectral confinement, mode hybridization, and significant near-field enhancement.

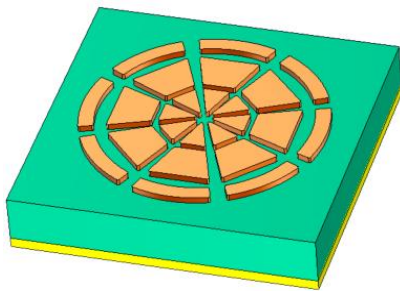


Fig. 1. Schematic of the proposed MMA.

The VO₂ segments possess a uniform height of 200 nm and the unit cell dimension is 56×56 μm². The analysis is based on finite element method (FEM) and the background material is considered air. The Drude model is applied to characterize the optical response of VO₂ in the THz frequency range [2]. Its dielectric function is given by:

$$\epsilon(\omega) = \epsilon_{\infty} - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} \quad (1)$$

Where $\epsilon_{\infty}=12$ represents the high-frequency dielectric permittivity, and $\gamma = 5.57 \times 10^{13}$ rad/s denotes the collision frequency. Simulating based on FEM, the MMA's reflectance and absorptance are evaluated and illustrated in Fig. 2. Periodic boundary conditions are applied along the x- and y-axes, while a perfect matching layer is considered in the z-direction at the impinging light side.

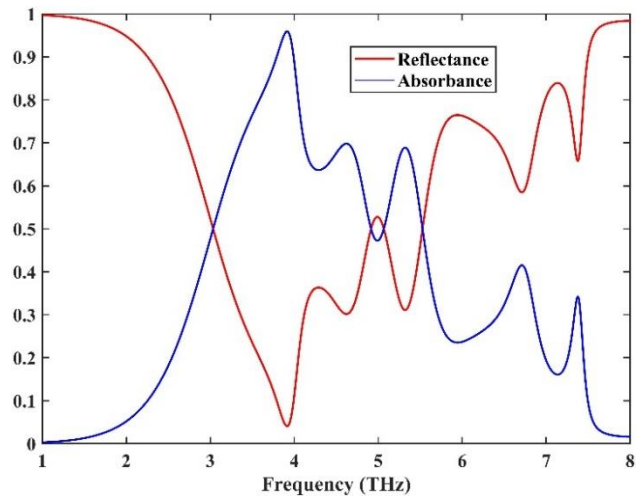


Fig. 2. Reflection and absorption for VO₂-based MMA in the frequency range of 1 to 8 THz.

The top view electric field distribution of the structure is illustrated in Fig. 3.

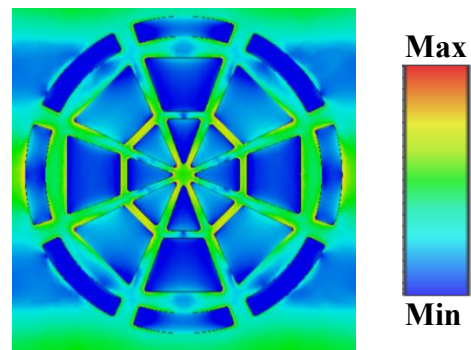


Fig. 3. The top view electric field distribution

References

1. Yang, Z., C. Ko, and S. Ramanathan, Oxide electronics utilizing ultrafast metal-insulator transitions. Annual Review of Materials Research, 2011. 41(1): p. 337-367.
2. P. Tonouchi, M., Cutting-edge terahertz technology. Nature photonics, 2007. 1(2): p. 97-105.

Didelio elektronų judrio tranzistorių su struktūriniais užtūros elektrodais taikymas terahercų spinduliuotės detekcijai / Modified Edge-Gating Geometry of High-Electron-Mobility Transistors for Terahertz Detection

Maxim Moscotin¹, Justinas Jorudas¹, Miroslav Saniuk¹, and Irmantas Kašalynas¹

1. Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius, email: maxim.moscotin@ftmc.lt

Terahertz (THz) technology has shown immense potential across various fields — including imaging, spectroscopy, and communication systems — but its full exploitation depends on the development of detectors. Terahertz antenna-coupled field-effect transistors (TeraFETs) have emerged as promising candidates for terahertz detection [1]. In these devices, resonant detection is achieved by exciting plasma waves within the transistor channel. The two-dimensional electron gas present in the channel acts as a plasmonic cavity, where interference of plasma waves results in resonant frequencies determined by the channel length and carrier density [2]. A critical challenge, however, is edge scattering. One promising approach to address this issue is to narrow the effective channel width electrically [3].

In this work, we developed TeraFETs based on AlGaIn/GaN high-electron-mobility transistor (HEMT) structures with an electrically controllable effective channel width. Three gate configurations are implemented: (i) an edge-configuration (EdgeFET), where two gate electrodes approach the channel from two sides; (ii) a modified edge-configuration (m-EdgeFET), in which the two side-approaching gates are interconnected by a small bridge overlapping the channel; and (iii) a reference configuration (FinFET) with a solid gate electrode fully covering the channel. Both gate and source-drain electrodes were implemented as perpendicular THz antennas, allowing operation of the detector in two regimes: direct channel coupling and capacitive coupling via gate electrodes. Compared to the reference FinFET, the m-EdgeFET geometry exhibits an order-of-magnitude reduction in gate leakage current and a similar magnitude of THz response. Furthermore, compared to the conventional EdgeFET, the m-EdgeFET shows a significantly lower threshold voltage of -3 V — an important factor for practical applications. The m-EdgeFET THz detector demonstrates room-temperature responsivity to 300 GHz, peaking at 13 V/W (Fig. 1).

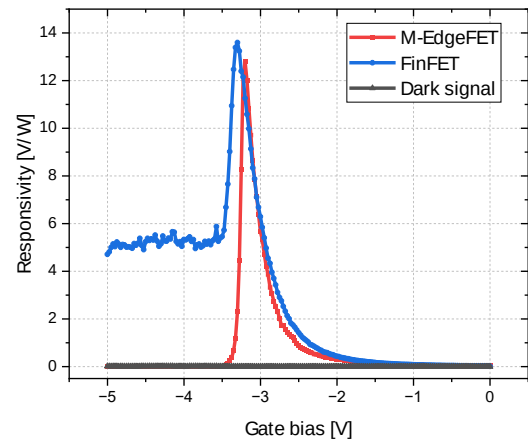


Fig. 1. Room-temperature responsivity to 300 GHz for an m-EdgeFET detector (red curve) and FinFET detector (blue curve) in an ohmic coupling regime.

Acknowledgement: the work received funding from LMT through the project: „Tyrimas bekausių žaliųjų technologijų GaN ir Ga₂O₃ galios įrenginiams gaminti naudojant lazerinį mikroapdorojimą“ (P-LT-TW24-1).

References

1. W. Knap et al., "Resonant detection of subterahertz and terahertz radiation by plasma waves in submicron field-effect transistors", *Applied Physics Letters*, vol. 81, no. 24, pp. 4637–4639, Dec. 2002.
2. Zhang Y. et al., "Resonant THz detection by periodic multi-gate plasmonic FETs", *Frontiers in Physics*, vol. 11, 1170265, 2023.
3. P. Sai et al., "AlGaIn/GaN field effect transistor with two lateral Schottky barrier gates towards resonant detection in sub-mm range", *Semicond. Sci. Technol.*, vol. 34, 024002, 2019.

THz spectroscopy of GeSn films for ultrafast optoelectronic applications

Simonas Driukas¹, Ričardas Norkus¹, Chia-Ming Mai², Cheng-Siang Le², Shang-Hua Yang²
and Gintaras Valušis³

1. Center for Physical Sciences and Technology, Department of optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius
2. National Tsing Hua University, Institute of Electronic Engineering, Dept. of EECS, Engineering III Building, 101 Sec. 1,
Kuang Fu Road, Hsinchu, Taiwan
3. Vilnius University, Faculty of Physics, Institute of Photonics and Nanotechnology, Saulėtekio av. 9, Vilnius email:
simonas.driukas@ftmc.lt

The growing demand for high-speed optoelectronic devices for photonic integration in computing, communications, security, and other fields has led to a search for low-cost, ultrafast semiconductors operating in the 1.55 μm optical range. One promising candidate in this regard is germanium-tin (GeSn). Pure germanium is an indirect-bandgap semiconductor; however, the incorporation of a few percent of tin lowers the energy of the Γ -valley, resulting in a smaller and direct bandgap [1]. Moreover, GeSn can be grown on silicon substrates via chemical vapor deposition, enabling industry-friendly fabrication and integration with existing Si platforms. The resulting GeSn layers can be further doped with ion-implanted phosphorus to reduce the carrier lifetime.

In this work, we are the first to employ terahertz (THz) spectroscopy techniques to characterize GeSn materials, revealing complex inter-valley dynamics and the ultrafast performance of doped GeSn..

1. THz excitation spectroscopy

Surface THz emission of GeSn samples was measured at different pump wavelengths to reveal the bandgap of the GeSn materials.

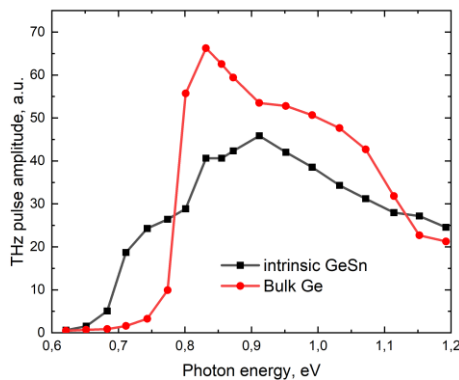


Figure 1. Surface excited THz emission amplitude with different pump photon energy.

A clear redshift can be observed comparing bulk Ge and GeSn samples.

2. Optical pump THz probe

Carrier dynamics were revealed by measuring the induced absorption changes via optical pump THz probe technique (OPTP).

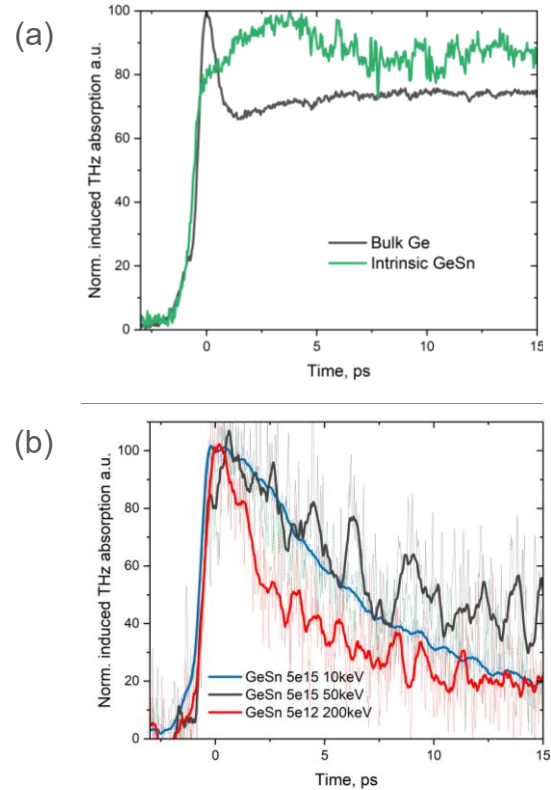


Figure 2. OPTP kinetics of (a) intrinsic Ge and GeSn, (b) doped GeSn. Dopant concentration and implantation energy is also displayed.

As expected, a substantial reduction in carrier lifetime is observed, caused by the formation of trapping centers associated with the implanted phosphorus atoms.

References

1. S. Ghosh, G. Sun, S. -Q. Yu and G. -E. Chang. *IEEE Journal of Selected Topics in Quantum Electronics*, vol. 31, no. 1, pp. 1-11, Jan.-Feb. 2025, Art no. 3800211.

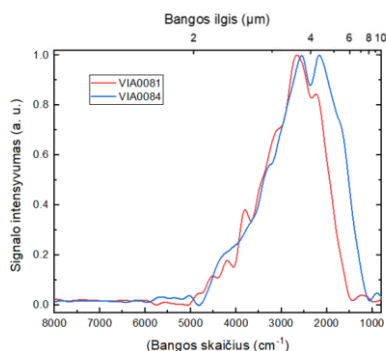
Stibidų pagrindo infraraudonosios spinduliuotės fotodetektoriai

Karolis Galvanauskas

Fizinių ir technologijos mokslų centras, Optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: karolis.galvanauskas@ftmc.lt

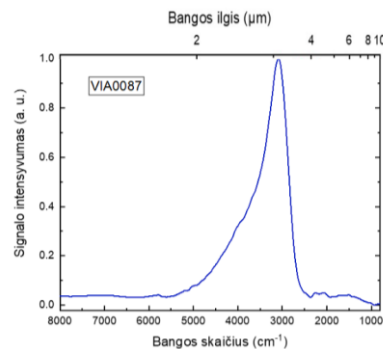
Ilgabangės infraraudonosios (LWIR) spinduliuotės detektorių rinkoje ilgą laiką dominuoja gyvsidabrio kadmio telurido (MCT) technologija. Tačiau gyvsidabrio toksiškumas skatina ieškoti našumu nenusileidžiančių, tačiau aplinkai saugesnių alternatyvų. Šiame pranešime pristatomi dviejų skirtingų stibidų pagrindu sukurtų fotodetektorių platformų kūrimo ir tyrimo rezultatai, kurie atveria kelią MCT detektorių pakeitimui.

Pirmasis metodas yra paremtas InAsSb trijų komponentų lydinio fotodiodais. Mūsų tyrimai parodė, kad molekulinio pluoštelio epitaksijos (MPE) metu tiksliai valdant As ir Sb srautų santykį (P_{Sb}/P_{As}) galima efektyviai keisti stibio (Sb) koncentraciją užaugintuose sluoksniuose nuo ~9% iki >20%. Fotoluminescencijos (PL) matavimai patvirtino, kad didėjant Sb kiekiui, draustinių energijų tarpas siaurėja ir pasiekia vertes, mažesnes nei 0.2 eV, o PL signalas nusidriekia į LWIR sritį, viršijančią 8 μm bangos ilgį (1 pav.). Ši platforma leidžia paprastai ir efektyviai derinti detektorių spektrinį jautrį.



1 pav. InAsSb bandinių (VIA0081-VIA0084) fotoluminescencijos spektrai, rodantys bangos ilgio poslinkį didinant Sb koncentraciją sluoksniuose.

Antrasis, sudėtingesnis metodas, naudoja InAs/GaSb II-o tipo supergardeles (T2SL). Šios heterostrukūros suteikia daugiau lankstumo projektuojant prietaisus ir leidžia pasiekti mažesnes tamsines sroves. MPE metodu sėkmingai užauginta sudėtinga 7 pakopų InAs/GaSb T2SL tarpjuostinio kaskadinio fotodetektoriaus (ICIP) struktūra (VIA0087). Didelės skiriamosios gebos rentgeno spindulių difrakcijos (HR-XRD) matavimais nustatytas supergirdelės periodas ($69 \pm 1 \text{ Å}$) idealiai atitiko projektinį (69 Å), kas patvirtina aukštą MPE proceso tikslumą. Kambario temperatūroje išmatuotas šio prietaiso fotovoltinis atsakas demonstravo itin stiprų signalą ties ~3.2 μm (2 pav.), kuris buvo apie 110 kartų stipresnis nei InAsSb struktūrų signalas. Tai įrodo efektyvų kaskadinio stiprinimo veikimą, nors atsako smailė ir neatitiko tikslinio LWIR dizaino, kas siejama su sandūrų įtaka ir aukštesnės eilės optiniais šuoliais.



2 pav. T2SL ICIP bandinio (VIA0087) fotovoltinio atsako spektras kambario temperatūroje, rodantis stiprų signalą MWIR srityje.

Apibendrinant, abi tirtos stibidų platformos – derinami InAsSb fotodiodai ir T2SL ICIP struktūros – demonstruoja didelį potencialą ateities IR jutiklių kūrimui ir yra perspektyvios, aplinkai saugios alternatyvos MCT technologijai.

Literatūra

1. E. A. Plis, Advances in Electronics 2014, 831397 (2014).
2. A. Rogalski, Infrared Physics & Technology 111, 103522 (2020).

Didelio pralaidumo erdvinė-laikinė optinė koherentinė tomografija

Austėja Trečiokaite

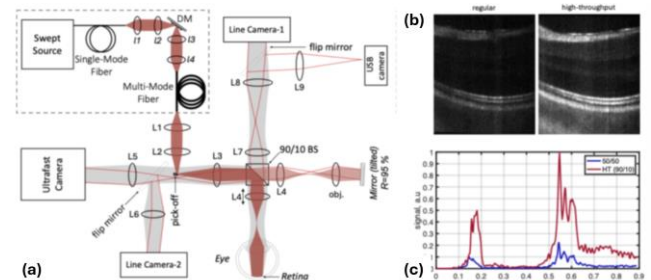
Fizinių ir technologijos mokslų centras, optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: austeja.treciokaite@ftmc.lt

Optinė koherentinė tomografija (OKT) vos per kelis dešimtmečius tapo kertiniu oftalmologinės diagnostikos metodu. Tačiau tradicinių skenuojančių sistemų galimybės tebėra ribojamos mažo skenavimo greičio bei judėjimo artefaktų. Eerdvinė-laikinė optinė koherentinė tomografija (ELOKT) leidžia atlikti didelės spartos tinklainės vaizdinimą, tačiau pasižymi ribotu jautriu. Šiame darbe pateikiame didelio pralaidumo (DP) optinę sistemą, kuri pagerina ELOKT jautrumą iki 3,5 karto (5,4 dB). Šis metodas išbandytas tiriant atspindinčius ir sklaidančius sintetinius bandinius bei *in vivo* žmogaus tinklainę. Gautas ryškus SNR pagerėjimas nedidinant šviesos šaltinio galios. Šis paprastas, šviesą taupantis metodas ELOKT padaro tinkamesnę realaus laiko, mažai atspindinčių, biologinių bandinių vaizdinimui. Tokie rezultatai pasiekti standartinį 50/50 pluošto daliklį pakeitus 90/10 dalikliu bei naudojant galinėje objektyvo židinio plokštumoje montuojamą nukreipiantį veidrodį, leidžiantį maksimaliai padidinti įeinančios šviesos ir signalo intensyvumą.

Naudojant įprastus 50/50 pluošto daliklius prarandama virš 75 % šviesos. Tai įvyksta dėl dvigubų nuostolių — apie 50 % šviesos prarandama apšvietimo metu ir dar tiek pat signalui grįžtant link kameros, be to, atskaitos atšakos atspindžio koeficientas turi būti labai žemas (tik keli procentai vaizdinant biomedicinius bandinius [1]), kas dar labiau padidina nuostolius. Paprasčiausiai padidinti šviesos šaltinio galią dažnai nėra galimybės, dėl šviesos šaltinio apribojimų arba fototoksinių efektų. Didelio pralaidumo (DP-) ELOKT pagerina SNR 3,5 karto, pakeičiant 50/50 pluošto daliklį į 90/10 bei naudojant nukreipiantį veidrodį apšvietimui ir detekcijai (1. pav. a). Šis sprendimas išnaudoja biologinių bandinių savybę tolygiai sklaidyti šviesą plačiais kampais. Nors simetriški 50/50 dalikliai vis vien geriau tinka stipriai atspindinčių bandinių, kuriems reikalingas didelis atraminis signalas, tyrimams, DP konstrukcijos žymiai pranašesnės vaizdinant silpnai atspindinčias, šviesą sklaidančias struktūras, tokias kaip žmogaus akies tinklainė.

Sistemos jautrumas buvo matuotas naudojant tiek 50/50, tiek 90/10 pluošto daliklius. Naudojant difrakcinę gardelę su 3,97 OD filtru ir slopinant atraminį veidrodį 0,6 OD, kad būtų užtikrintas šratinio triukšmo ribojamas veikimas, jautrumas siekė 81,2 dB esant įprastinei konstrukcijai ir 86 dB DP režimui — tai reiškia 2,8 karto (4,5 dB) padidėjimą vienam registruojamų vaizdų paketui ir net iki 3,5 karto (5,4 dB) pagerėjimą vidurkinant 30 vaizdų paketų [2]. *In vivo* tinklainės tyrimas patvirtino SNR pagerėjimą: ašinės ELOKT projekcijos atskleidė tinklainės sluoksnius struktūras, matomas tik DP režimu (1 pav. b, c). Skirtingai nei ankstesniuose bandymuose, šie rezultatai gaunami dėl didesnio šviesos kiekio ateinančio iš bandinio, o ne dėl tamsaus lauko efektų [3]. Nors poliarizuojantys pluošto dalikliai su ketvirčio bangos ($\lambda/4$) plokštelėmis [4] taip

pat galėtų padidinti šviesos pralaidumą link ir nuo bandinio, tačiau naudojant nepoliarizuotus šviesos šaltinius (multimodinių šviesolaidžių apšviečiama ELOKT) automatiškai būtų prarandama pusė šaltinio generuojamos šviesos bei netiktų dvejopalaui bandiniams ir atspindžių slopinimui.



1 pav. (a) Darbe naudotos sistemos principinė schema. Rezultatų, gautų atliekant *in vivo* tinklainės tyrimą su standartinėmis (b, c, mėlyna kreivė) ir didelio pralaidumo ELOKT sistema (b, c, raudona kreivė) palyginimas.

Literatūra/References:

1. A. Dubois, L. Vabre, A. C. Boccara, and E. Beaufort, "High resolution full-field optical coherence tomography with a Linnik microscope," *Appl. Opt.* 41, 805-812 (2002).
2. K. Adomavicius, A. Trečiokaite, E. Tarvydas, and E. Aukorius, "High-throughput spatio-temporal optical coherence tomography (STOC-T)," *Optics Continuum*, Aug. 2025, doi: 10.1364/optcon.564109.
3. E. Aukorius, and A. C. Boccara, "High-throughput dark-field full field optical coherence tomography," *Optics letters* 45, 455-458 (2020).
4. P. Balondrade, V. Barolle, N. Guigui, E. Auriant, N. Rougier, C. Boccara, M. Fink, and A. Aubry, "Multi-spectral reflection matrix for ultrafast 3D label-free microscopy," *Nature Photonics* 18, 1097-1104 (2024).

CILINDRINĖS REZONANSINĖS ANTENOS RADIO BANGŲ ENERGIJOS RINKIMUI

Justina Žemgulytė

Fizinių ir technologijos mokslų centras, Fizikinių technologijų skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: justina.zemgulyte@ftmc.lt

Mikrobangų ir milimetrinių bangų technologijų plėtra reikalauja kompaktiškų, efektyvių ir lengvai integruojamų antenų. Dielektrinės rezonansinės antenos (DRA) dėl savo konstrukcijos paprastumo ir ypač mažų elektromagnetinių nuostolių vis plačiau yra pritaikomos radijo bangų energijos rinkimui.

Dažniausiai DRA cilindras žemės plokštumos atžvilgiu yra orientuojamas vertikaliai. Šiame darbe siūloma horizontali antenos orientacija (1 pav.). Tokia antena turi du apskritus metalinius kontaktus, vienas jų sujungtas su koaksialinės jungties karštu kontaktu, o kitas – prie žemės plokštumos, ant kurios paguldytas dielektrinis cilindras.

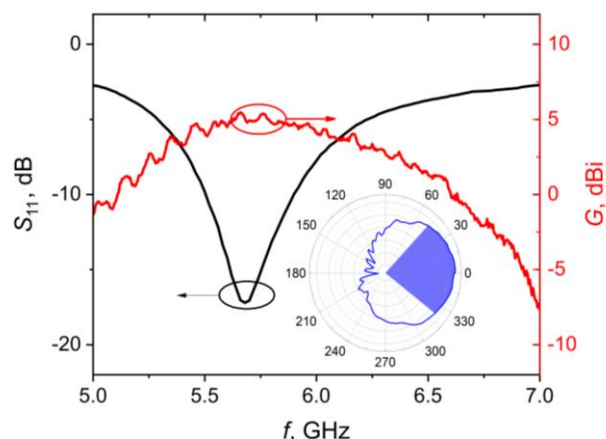
Eksperimentiškai ir teoriškai ištirtos trys antenos, veikiančios šiais centriniais dažniais: 5,75 GHz, 2,4 GHz ir 1,575 GHz. Jos pagamintos iš dielektrinių cilindrių, kurių dielektrinė skvarba buvo atitinkamai 32, 17 ir 12. Modeliavimas, naudojant CST Studio, parodė, kad antena spinduliuoja statmenai žemės plokštumai, o didžiausias realizuotas stiprinimas siekia apie 6 dBi. Eksperimentiniai matavimai su kompozitiniais keraminiais bandiniais susintetintais Kijevo V. I. Vernadskio bendrosios ir neorganinės chemijos institute patvirtino modeliavimo rezultatus. Antenos, pagamintos iš susintetintos keramikos $0.93(\text{Mg}_{0.97}\text{Ni}_{0.05})\text{TiO}_3 \cdot 0.07\text{Ca}_{0.8}\text{Sm}_{0.13}\text{TiO}_3$ su $\epsilon_r = 17$ ir veikiančios 5,75 GHz dažnyje, matavimo rezultatai pateikti 2 pav. Antena pasiekia apie 5,5 dBi maksimalų stiprinimą ties 5,7 GHz, o atspindžio koeficientas yra mažesnis nei -10 dB. Spinduliavimo diagramoje matyti, kad antena spinduliuoja plačiu kampu – pusės galios spindulys išmatuotas apie 70 laipsnių. Matavimo rezultatai patvirtina, kad ši antena gali būti naudojama radijo bangų energijos rinkimui: dažnių juosta apima 5 GHz Wi-Fi ruožą, 6 dBi stiprinimas užtikrina didelę surenkamos energijos dalį, o platus spinduliavimo kampas leidžia rinkti energiją iš įvairių krypčių.

Buvo atlikti preliminarūs radijo bangų energijos rinkimo matavimai. Tam buvo pagamintas vienos pakopos įtampos lygintuvas ir jam pritaikytas impedanso derinimo grandynas, pasiekiantis atspindžio koeficientą žemiau -10 dB ties 5,7 GHz. Įtampos lygintuvo efektyvumas buvo matuojamas



1 pav. Cilindrinės dielektrinės antenos iliustracija

esant 1 mW įėjimo galiai, 3 kΩ apkrovai ir 5,7 GHz



2 pav. Cilindrinės dielektrinės rezonansinės antenos matavimo rezultatai (raudona linija – stiprinimas, juoda linija – atspindžio koeficientas, mėlyna linija – spinduliavimo diagrama).

dažniui. Gautas efektyvumas siekė apie 16 %, o išėjimo įtampa buvo 690 mV. Dielektrinė antena kartu su lygintuvu galėjo surinkti 16 μW galios, kai mikrobangų šaltinio galia buvo 150 mW, o atstumas iki jo – 1 metras.

Kaip ir literatūroje [1], buvo pasiektas ribotas efektyvumas dėl diodų nuostolių aukštuose dažniuose. Vienas iš būdų spręsti šią problemą – rinkti žemesnio dažnio radijo bangų energiją, pavyzdžiui, Wi-Fi 2,4 GHz ruože. Šios antenos paprasta konstrukcija taip pat leidžia apsvarstyti galimybę konstruoti antenų masyvus. Modeliuojant patvirtinta, kad dviejų antenų masyvas gali pasiekti apie 9 dBi stiprinimą. Matavimai rodo, kad antena gali būti naudojama radijo bangų priėmimo sistemose, belaidžio ryšio tinkluose, MIMO sistemose ir kitose srityse, kur reikalingas platus spinduliavimo kampas ir kompaktiškas dizainas.

Šį tyrimą rėmė NATO Mokslo taikai ir saugumui programa, projektas G6002 „3D metamedžiagos energijos surinkimui ir mikrobangų matavimams“.

Literatūra

- [1] M. Mattsson, C. I. Kolitsidas, and B. L. G. Jonsson, 'Dual-Band Dual-Polarized Full-Wave Rectenna Based on Differential Field Sampling', *Antennas Wirel. Propag. Lett.*, vol. 17, no. 6, pp. 956–959, June 2018, doi: 10.1109/LAWP.2018.2825783.

OPTICAL PROPERTIES OF *trans*-STILBENE IN DIFFERENT PHASES: MONOMERS, AGGREGATES AND CRYSTALLITES

Ivan Halimski¹, Andrej Dementjev¹, Jevgenij Chmeliov^{1,2}, Mindaugas Mačernis², Darius Abramavičius², Leonas Valkūnas¹, Renata Karpicz¹

1. Center for Physical Sciences and Technology, Department of Molecular Compound Physics
Saulėtekio av. 3, LT-10257 Vilnius, email: ivan.halimski@ftmc.lt
2. Vilnius University, Faculty of Physics, Institute of Chemical Physics
Saulėtekio av. 9-III, LT-10222 Vilnius

Stilbene is an organic compound with structural formula $C_6H_5CH=CHC_6H_5$ ($C_{14}H_{12}$), the most well-known feature of which is *cis-trans* photoisomerization under ultraviolet irradiation. That is why stilbene plays an important role in physics, chemistry and biology. However, *trans*-isomer, which is solid crystal in ambient conditions, is more stable than the *cis*- one, which is a liquid.

Trans-stilbene (TS) itself is used for sensing and screening applications, as well as for neutron detection. Recently, it was shown that TS is able to form quite stable van der Waals complex with hexagonal boron nitride [1], and this might open a new scope of possible applications of TS and/or its derivative compounds. For example, TS derivatives resveratrol and pterostilbene demonstrate anti-cancer and antifungal activities.

Bulk TS is known to exhibit unusual temperature dependence of its optical properties [2]. However, despite the broad interest and a big scope of applications, TS thin films containing different species are not deeply studied and their optical properties are not completely understood.

To fill this gap, we studied optical properties of TS thin films in polystyrene (PS) matrix varying both TS concentration with respect to PS mass (from 0.5% to 80%) and thickness of the films (from 45 nm to 670 nm). We utilized coherent anti-Stokes Raman scattering (CARS) and atomic force microscopy (AFM) in order to study the structure of the films and UV/vis absorption as well as steady-state fluorescence (FL), FL excitation spectra and FL decay kinetics to understand their optical properties.

We discovered, that TS thin films exhibit smooth transition of FL properties from monomeric ones to the properties of disordered aggregates [3, 4] with quenched FL and, for higher concentrations, to the properties of structured nano-crystallites [4]. Additionally, we performed temperature-dependent (from 15K to 290K) steady-state FL and FL decay kinetics measurements to discover specific properties of all the TS species.

References

1. I. Halimski, et. al., Langmuir 41, 11, 7364 (2025).
2. R. Karpicz, et.al., Phys. Chem. Chem. Phys. 23, 3447 (2021).
3. R. Karpicz, et.al., Phys. Chem. Chem. Phys. 25, 21183 (2023).
4. I. Halimski, et.al., Phys. Chem. Chem. Phys. 26, 23692 (2024).

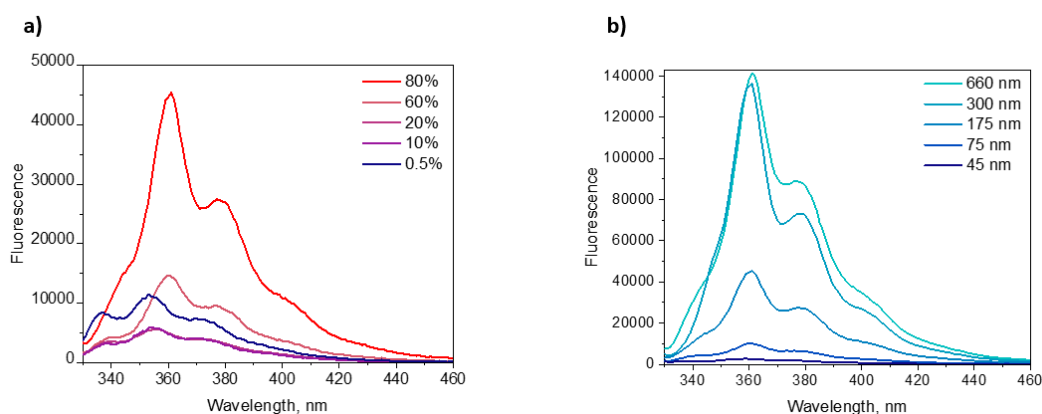


Fig. 1. a) Concentration-dependent FL at the fixed 175 nm thickness and b) thickness-dependent FL at the fixed 80% concentration.

Rational Design of Molecularly Imprinted Polymer for Melamine and Cyanuric Acid Detection: A DFT Approach

Enayat Mohsenzadeh¹, Vilma Ratautaite¹, Arunas Ramanavicius¹

1. Centre for Physical Sciences and Technology, Department of Nanotechnology

Saulėtekio av. 3, LT-10257 Vilnius, email: enayat.mohsenzadeh@ftmc.lt

Molecularly imprinted polymers (MIP) are synthetic receptors with tailor-made binding sites for a specific target. The MIP synthesis has a stepwise process including (1) the selection of optimal pre-polymerisation reagents, (2) polymerisation, (3) extraction of template (target) molecules from the polymer film, and (4) rebinding of target molecules on the MIP. As a result, a functional polymer film comprising binding sites is created that empower MIPs to detect the target selectively 1.

However, the selection of reagents and methods intensely impacts the MIP recognition performance. Therefore, the MIP preparation process requires exhaustive trial-error experiments, which are time-consuming, expensive and ecologically destructive. Computational methods can minimise the need for experiments. Once optimal condition is provided, the smarter design of MIPs is feasible which leads to better experiment results 2. The atomistic level of simulations along with quantum mechanical calculations are widely used for the MIP design.

Density functional theory (DFT) calculations were applied to design the MIP for simultaneous detection of

melamine and cyanuric acid in this study. The selection of the best functional monomer was done for achieving the highest affinity. Then, the optimal molar ratio of monomer to template was calculated. The candidate solvents were assessed and the study of MIP interactions with the target was evaluated. Surface analyses demonstrated the imprinting efficiency of binding sites.

References

1. G. Zvirzdine, S. Zukauskas, A. Rucinskiene, E. Mohsenzadeh, R. Boguzaite, A. Ramanaviciene, M. Pogorielov, V. Ratautaite, A. Ramanavicius, Electrochemical Salicylic Acid Sensor Based on Molecularly Imprinted Polypyrrole, ACS Appl. Mater. Interfaces (2025).
2. E. Mohsenzadeh, V. Ratautaite, E. Brazys, S. Ramanavicius, S. Zukauskas, D. Plausinaitis, A. Ramanavicius, Design of molecularly imprinted polymers (MIP) using computational methods: A review of strategies and approaches, WIREs Computational Molecular Science 14 (2024) e1713.

NiZn/Ti and Au(NiZn)/Ti Anode catalysts for Borohydride Oxidation in Clean Energy Systems

Tripura Ganti¹, Aldona Balčiūnaitė¹, Jūrate Vaičiūnienė¹, Loreta Tamašauskaitė-Tamašiūnaitė¹, Eugenijus Norkus¹

1. Department of Catalysis, Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania
tripura.ganti@ftmc.lt

Direct borohydride fuel cells (DBFCs), a subgroup of alkaline fuel cells, are among the most attractive options for clean energy applications. However, they require suitable anode catalysts for efficient borohydride oxidation (BOR). Although noble metals act as effective catalysts for BOR, their scarcity limits large-scale applications. Therefore, in this work, we developed pure non-noble NiZn/Ti electrodes, as well as Au-modified NiZn/Ti electrodes with the deposited gold loading of 20 $\mu\text{g}_{\text{Au}} \text{cm}^{-2}$, as anode catalysts for BOR.

The NiZn/Ti electrodes were fabricated via single-step electrodeposition using the electrochemical bath consisting of 0.2 M Ni^{2+} , 0.2 M Zn^{2+} , 0.2 M H_3BO_3 , and 0.2 M $(\text{NH}_4)_2\text{SO}_4$, pH 2.8. Electrodeposition was carried out at 25 °C under a constant current of 1 A for 1 minute, followed by alkaline leaching for 48 hours and gold galvanic displacement in HAuCl_4 solution for 1 minute. Zn leaching produced dendritic surface morphologies, whereas the introduction of a low Au loading on the NiZn/Ti electrode increased surface roughness and enhanced the number of active catalytic sites. The BOR activity of the prepared catalysts was

evaluated using cyclic voltammetry in various concentrations of NaBH_4 , with 1 M NaOH as the supporting electrolyte, in the potential range of 0.2 V to –0.6 V (vs. SCE), at a scan rate of 10 $\text{mV} \cdot \text{s}^{-1}$.

Electrochemical measurements showed that NiZn/Ti drives BOR at more positive potentials, whereas Au incorporation shifts the activity toward more negative potentials. The anodic peak current densities for borohydride oxidation increased linearly with the square root of the scan rate for both NiZn/Ti and Au(NiZn)/Ti electrodes, indicating a diffusion-controlled process.

The peak currents increased with BH_4^- concentration (0.01–0.05 M) and were consistently higher for the Au(NiZn)/Ti electrode, demonstrating that Au incorporation enhances catalytic activity and electron transfer efficiency. Higher electrolyte concentrations further improved BOR performance. Kinetic analysis confirmed a diffusion-controlled reaction mechanism.

These results establish NiZn/Ti and Au(NiZn)/Ti as efficient and durable anode catalysts for DBFC applications.

Bismuth-Doped Laser-Induced Graphene Electrodes for Simultaneous Detection of Zn^{2+} , Pb^{2+} , and Cd^{2+}

Pamela Rivera¹, Annalisa Scroccarello², Ida Valeria Di Cristoforo², Davide Paolini², Dario Compagnone², Rasa Pauliukaite¹, Flavio Della Pelle²

1. Center for Physical Sciences and Technology, Department of Nanoengineering
Savanoriu Ave. 231, LT-02300 Vilnius, Lithuania

2. Department of Bioscience and Technology for Food, Agriculture and Environment, University of Teramo, via R. Balzarini 1, 64100 Teramo, Italy. email: pamela.rivera@ftmc.it

Heavy metals (HMs) are among the main environmental pollutants affecting ecosystems and human health [1]. They accumulate in soils and water bodies due to industrial activity, mining, and agricultural runoff. Once present, they persist and interfere with biological systems by damaging membranes, disrupting enzymes, and altering genetic material [2].

Biological approaches such as phytoremediation (using plants) and biosorption/bioaccumulation (using microbes) offer a sustainable and low-cost strategy to reduce HM contamination [3]. However, assessing their effectiveness still relies on centralized and expensive laboratory techniques. Electrochemical sensors are a promising alternative: they are accurate, portable, and robust. Yet, complex material fabrication continues to limit their scalability and practical use for in-field environmental monitoring.

In this work, we explore bismuth-doped laser-induced graphene (Bi-LIG) as a sensing platform for the simultaneous detection of Zn^{2+} , Pb^{2+} , and Cd^{2+} at trace levels using square wave anodic stripping voltammetry (SWASV). Bi-LIG is made through a single-step laser process using a polyimide film coated with a bismuth-PVA hydrogel ink. The fabrication is fast, low-cost, and scalable.

The resulting material combines the mechanical flexibility and porosity of LIG with the electrocatalytic properties of bismuth nanoparticles, making it a strong candidate for in-field sensing [4]. The quality of the graphene was evaluated with Raman spectroscopy, while SEM-EDS and XPS were used to study the composition and distribution of the laser-formed bismuth nanoparticles. Electrochemical characterization was performed using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). Finally, the electrode's performance in detecting Zn^{2+} , Pb^{2+} , and Cd^{2+} will be assessed.

This work presents a practical alternative for the scalable and field-deployable electrochemical detection of heavy metals in agriculture.

References

1. Tchounwou, P. B. et al. Heavy metal toxicity and the environment. *EXS* 101, 133–164 (2012).
2. Jaishankar, M. et al. Toxicity, mechanism and health effects of some heavy metals. *Interdiscip. Toxicol.* 7, 60–72 (2014).
3. Ali, H., Khan, E., & Sajad, M. A. Phytoremediation of heavy metals—Concepts and applications. *Chemosphere*, 91(7), 869–881 (2013).
4. Novosselov, I. V. et al. Laser-induced graphene: a new tool for electrochemical sensing. *ChemElectroChem* 7, 2039–2050 (2020).

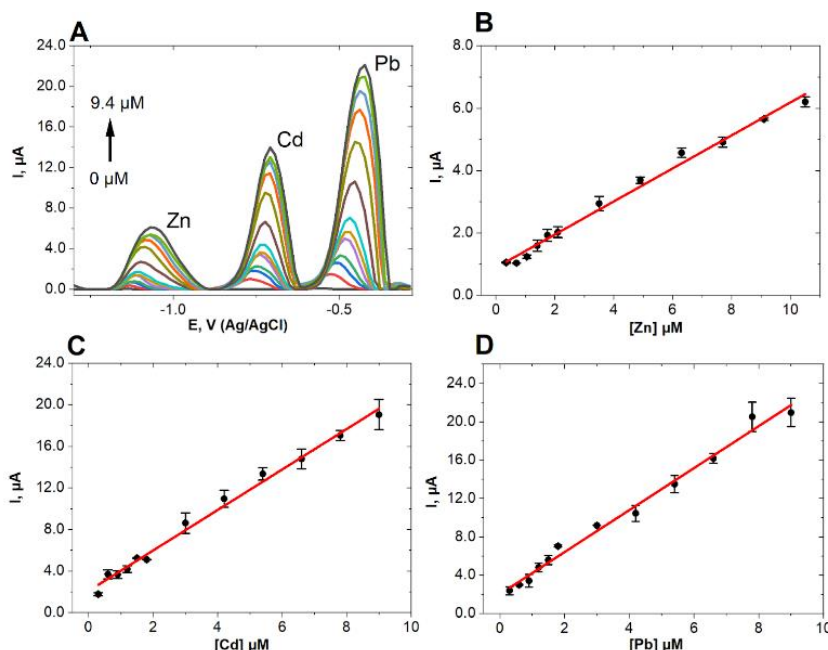


Figure 1. (A) Voltammograms obtained using SWASV at increasing analyte concentrations. (B–D) Calibration curves for Zn^{2+} , Cd^{2+} , and Pb^{2+} .

Heavy metal sensing capabilities of MXenes and potential applications in protein detection

Ilya Navitski¹, Šarūnas Žukauskas¹, Simonas Ramanavičius¹, Alma Ručinskienė¹, Arūnas Ramanavičius^{1,2}

1. State Research Institute Center for Physical Sciences and Technology (FTMC), Sauletekio Av. 3, LT-10257 Vilnius, Lithuania

2. Faculty of Chemistry and Geosciences, Vilnius University (VU), Naugarduko g. 24, LT-03225 Vilnius, Lithuania
email: ilya.navitski@ftmc.lt

MXenes are a family of 2D nanomaterials with advantageous properties for developing sensing platforms. Their electrical conductivity is comparable to that of graphene; however, unlike graphene, MXenes possess tunable surface termination groups, which facilitate easier functionalization. They are significantly less expensive than other 2D nanomaterials, making their use in sensor construction more practical and cost-effective [1]. In addition, their large surface area, unique optical characteristics, and biocompatibility enable MXenes to be applied for various sensing strategies for a wide range of targets [2,3]. In this work, we developed a reliable and accurate MXene-based electrochemical sensor for cadmium ion detection in aqueous solutions. We also investigated effects of MXenes addition to electrode structure for potential biosensing applications.

For cadmium sensing, a glassy carbon electrode (GCE) was modified by drop-casting MXenes–Nafion composites. Sensor performance was evaluated using differential pulse voltammetry (DPV). All cadmium-related experiments were conducted in acetate buffer at pH range from 3.5 to 5.5 and temperatures ranging from 8 to 30 °C. Biosensor-related experiments were carried out in 2.5 mM K₄[Fe(CN)₆]/K₃[Fe(CN)₆] solution prepared in phosphate buffer, using an indium tin oxide (ITO) platform modified with either (3-aminopropyl)triethoxysilane (APTES) alone or MXenes–APTES.

The cadmium sensor demonstrated selective detection in the presence of various ions. Lead ions could also be detected without interference between cadmium and lead signals. Both pH and temperature influenced sensing performance: acidic conditions improved sensitivity but narrowed the working range, while higher temperatures enhanced detection at the cost of potential MXenes oxidation. At pH 4.5 and 22 °C, the sensor achieved a limit of detection (LOD) of 0.82 μM and a sensitivity of 5.11 ± 0.08 μA/(μM·cm²) within the 1.03–27.53 μM range. Electrode performance gradually declined over time, though it remained relatively stable for the first three weeks. The method was successfully applied to real water samples (Fig. 1), yielding recovery rates between 97.18% and 108.40% for Sudervė Lake compared to ICP-MS.

Regarding biosensor applications, incorporating MXenes into the APTES-ITO structure significantly enhanced electrochemical performance compared to the APTES-modified ITO without MXenes, highlighting MXenes-APTES as a promising platform for biosensor development.

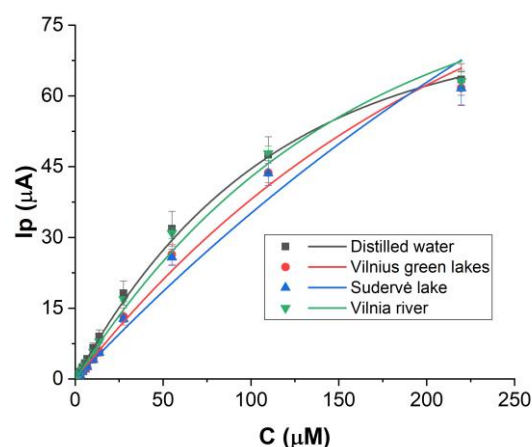


Fig. 1. Concentration curve of cadmium ion sensing (n=3) in different aqueous environments.

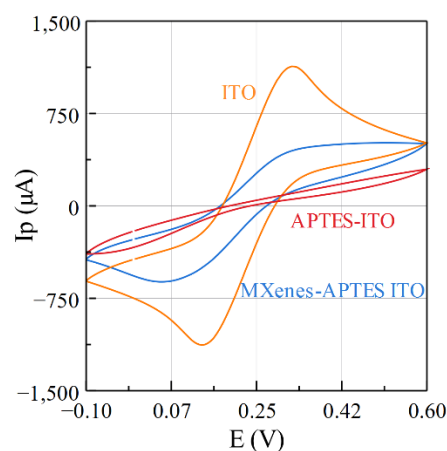


Fig. 2. Comparison between electrochemical performance of modified and unmodified ITOs.

References

- Ilya Navitski et al. 2D MXenes in the design of heavy metal ion sensors (review) (Trends in Environmental Analytical Chemistry, 47, 2025).
- Ilya Navitski et al. MXene-Based Chemo-Sensors and Other Sensing Devices (Nanomaterials, 14, 2024).
- Sarunas Zukauskas et. al Electrochemical real-time sensor for the detection of Pb(II) ions based on Ti₃C₂T_x MXene (Science of The Total Environment, 950, 2024).

Comparative study of amino acids influence on the hydrothermally synthesized CoFe_2O_4 nanoparticles

Aswathi Raveendran¹, Germante Paulikaite¹, Agne Mikalauskaitė¹, Vidas Pakstas¹, Kestutis Mazeika¹,
Jurate Vaiciuniene¹, Arunas Jagminas¹, Simonas Ramanavicius¹

1. Center for Physical Sciences and Technology, Department of Electrochemical Materials Research

Saulėtekio av. 3, LT-10257 Vilnius, email: aswathi.raveendran@ftmc.lt

Magnetic nanoparticles are extensively studied at the nanoscale for applications in data storage, magneto-optical devices, and biomedicine [1,2,6]. Among ferrites, cobalt ferrite (CoFe_2O_4) is of particular interest due to its high. The properties of CoFe_2O_4 are strongly influenced by particle size, morphology, and surface characteristics, which in turn are determined by the synthesis method. Techniques such as hydrothermal, sol-gel, and co-precipitation are commonly employed, where reaction parameters including temperature, stirring speed, and pH govern the balance between nucleation and growth [3,4,5]. A major challenge in synthesizing magnetic nanoparticles is their tendency to agglomerate, driven by high surface energy and magnetic interactions. While surface modification can reduce this effect, surfactants offer an efficient approach by introducing electrostatic repulsion and steric hindrance. This not only minimizes aggregation but also enhances control over nucleation and growth, enabling the optimization of crystallite size, porosity, and surface area [6].

In this study, CoFe_2O_4 nanoparticles were synthesized by the hydrothermal co-precipitation method with and without amino acids, which work as capping agents [2,7]. The influence of amino acids on the structural and magnetic properties of the nanoparticles was investigated with the aim of tuning the stability and performance. The findings of this study contribute to the development of highly stable CoFe_2O_4 nanoparticles and highlight their potential application as magnetically separable adsorbents and catalysts for wastewater treatment.

Acknowledgment: This project received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-24-14.

References

1. S.M. Ansari, B.B. Sinha, K.R. Pai, S.K. Bhat, Y.R. Ma, D. Sen, Y.D. Kolekar, C.V. Ramana, Controlled Surface/Interface Structure and Spin Enabled Superior Properties and Biocompatibility of Cobalt Ferrite Nanoparticles. *Appl. Surf. Sci.* 2018, 459, 788-801.
2. R. Žalneravičius, A. Mikalauskaitė, G. Niaura, A. Paškevičius, A. Jagminas, Ultra-small methionine-capped AuO/Au^+ nanoparticles as efficient drug against the antibiotic-resistant bacteria. *Mater Sci Eng C Mater Biol Appl.* 2019, 102, 646-652.
3. Sukoviene, S. Ali, A. Jagminas, S. Ramanavicius, Magnetic Cobalt and Other Types of Ferrite Nanoparticles: Synthesis Aspects and Novel

Strategies for Application in Wastewater Treatment (Review). *Appl. Sci.* 2025, 15(2), 857.

4. M. Plečkaitis, V. Karabanovas, G. Butkiene, J. Venius, M. Burkanas, G. Grinciene, A. Jagminas, R. Rotomskis, Magnetic Nanoparticles Decorated with Gold Nanoclusters-Applications in Cancer Theranostics. *Adv. Mater. Interfaces*, 2023, 10, 1-12.
5. Shyamaldas, M. Bououdina, C. Manoharan. Dependence of structure morphology on electrical magnetic properties of hydrothermally synthesised cobalt ferrite nanoparticles. *J. Magn. Magn. Mater.* 2020, 493, 165703.
6. M. Kurtinaitiene, K. Mazeika, S. Ramanavicius, V. Pakstas, A. Jagminas, Effect of Additives on the Hydrothermal Synthesis of Manganese Ferrite Nanoparticles. *Adv. Nano. Res.* 2016, 4, 1-14.
7. K. Sangsuriyong, N. Paradee, K. Rotjanasuworapong, et al. Synthesis and characterization of $\text{Co}_{1-x}\text{Fe}_x\text{Fe}_2\text{O}_4$ nanoparticles by anionic, cationic, and non-ionic surfactant templates via co-precipitation. *Sci Rep*, 2022, 12, 4611.

AU FUNCTIONALIZED MXENE FOR PLASMONIC DETECTION OF ORGANIC MOLECULES IN WATER

Saqib Ali¹, Martynas Talaikis¹, Oleksiy Gogotsi², Arunas Jagminas¹, Simonas Ramanavicius¹

1. Materials Research Center LLC, Carbon-Ukraine (Y-Carbon Ltd.)
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: saqib.ali@ftmc.lt

Colorimetric sensors are gaining popularity in biological and environmental sensing, because they are easy to use, cost effective, and fast. These are highly sensitive and selective, these qualities making them useful for detecting different substances in aqueous medium. They can be used to detect both organic and inorganic analytes in water, such as pharmaceuticals, proteins, amino acids, viruses, and inorganic pollutants in waters such as heavy metal ions [1][2]. Colorimetric sensors are sensitive to concentration and show a visible change in color with respect to analyte concentration, enabling real-time and highly sensitive analysis. However, these sensors face limitations, such as a low extinction coefficient and poor accuracy. [3]. Advanced nanomaterials, including 2D materials, metal oxide nanoparticles, and quantum dots, can significantly improve colorimetric sensors' performance and capabilities [4]. MXene is the latest addition to the 2D material family. Since their discovery back in 2011, have gained significant attention for their versatile applications, due to their high surface area and chemical tunability [5]. We present an Au nanocluster decorated MXene-based colorimetric sensor developed at room temperature for the colorimetric detection of tiny quantities of pharmaceuticals in water. In this study, we decorate MXene with Au nanoclusters, which show an evident plasmonic effect at 590 nm due to the local surface plasmonic resonance (LSPR) effect. We used this Au-

modified MXene as an optical probe for sensing of the analyte. We demonstrated the use of Au-modified MXene for the detection of the emerging pollutant paracetamol. The work shows the linear response between the change of paracetamol concentration in water and the change in plasmonic response of Au modified MXene, with high detection sensitivity and selectivity. Furthermore, our work broadens the use of MXene in colorimetric sensor technology and provides a simple analyte sensing platform, opening a new route for extremely versatile colorimetric sensors for future applications.

References:

1. S. Zukauskas et al., Electrochemical real-time sensor for the detection of Pb(II) ions (Sci. Total Environ., vol. 950, p. 175190, Nov. 2024).
2. I. Navitski, A. Ramanaviciute, S. Ramanavicius, M. Pogorielov, and A. Ramanavicius, MXene-Based Chemo-Sensors and Other Sensing Devices, (Nanomater. 2024, Vol. 14, Page 447, vol. 14, no. 5, p. 447, Feb. 2024)
3. J. Zhou et al., Recent Advances in Design and Application of Nanomaterials-Based Colorimetric Biosensors for Agri-food Safety Analysis (ACS Omega, vol. 8, no. 49, pp. 46346–46361, Dec. 2023)
4. Y. Wu et al., Colorimetric Sensors for Chemical and Biological Sensing Applications, (Sensors 2023, Vol. 23, Page 2749, vol. 23, no. 5, p. 2749, Mar. 2023)
5. M. Naguib et al., Two-Dimensional Nanocrystals Produced by Exfoliation of Ti₃AlC₂, (Adv. Mater., vol. 23, no. 37, pp. 4248–4253, Oct. 2011)

MAGNETIC FIELD DYNAMICS DURING MAGNETIC PULSE FORMING AND CRIMPING

Pavel Piatrou¹, Voitech Stankevič¹, Skirmantas Keršulis¹, Vilius Vertelis¹, Nerija Žurauskienė¹

1. Center for Physical Sciences and Technology, Department of Functional Materials and Electronics
Saulėtekio av. 3, LT-10257 Vilnius, email: pavel.piatrou@ftmc.lt

The utilization of pulsed magnetic fields in the welding and crimping of metals constitutes a contemporary, eco-friendly technique that eliminates the need for mechanical pressure. This process involves the use of short, high-amplitude, pulsed magnetic fields, and the analysis of these dynamics provides significant insights into the assessment of quality and the optimization of the process. This study proposes a computerized fast magnetic field measurement system that facilitates precise measurements of pulsed magnetic fields reaching up to 15 T with 32 μ s duration.

To study the magnetic field dynamics in magnetic pulse crimping and welding, we upgraded our setup consisting of new 50 μ F capacitors and a new 5-turn Bitter coil. The setup allows for short pulsed magnetic fields, which we recorded with a fast B-scalar meter (Fig. 1). We conducted a series of experiments and compared them with a result obtained at the previous setup.

We investigated how the presence of aluminum rods and tubes affects the magnetic field in the field shaper of Bitter coil at different discharge energies.

At first stage we study the dynamics of the magnetic field during pulse formation and flyer compression with an energy of 1.6 kJ, four consecutive experiments were conducted and then compared with each other (Fig.2).

The characteristics obtained using the new Fast B-scalar measurement system make it possible to precisely determine the onset time of the flyer's plastic deformation as well as the moment of impact with the parent part.

The time from the onset of plastic deformation to impact with the rod is approximately 4 microseconds at an energy of 1.6 kJ. Analysis of the first peak's dynamics of aluminum 6063 tubes shows that the welding or crimping process is completed during the first peak of the magnetic field.

Experiments with flyer-tubes of various wall thicknesses w and parent rod diameters D (Fig. 3) revealed the possibility of using the sensor as a proximity detector based on the second peak of the damped signal. This feature becomes useful for analyzing the final results of magnetic pulse welding of thin-walled tubes, where indentation of the parent tube may occur upon impact.

On the upgraded setup, we also obtained first our welding results of aluminum 1060 tubes and stainless steel 304 rods. To validate these results, peel tests were conducted on the specimens.

The fast B-scalar measuring device with colossal magnetoresistance sensors, has the potential to become a decisive system for investigating the dynamics of magnetic pulse crimping, welding, and forming processes. At this time, this system is a unique tool to advance research and industrial applications.

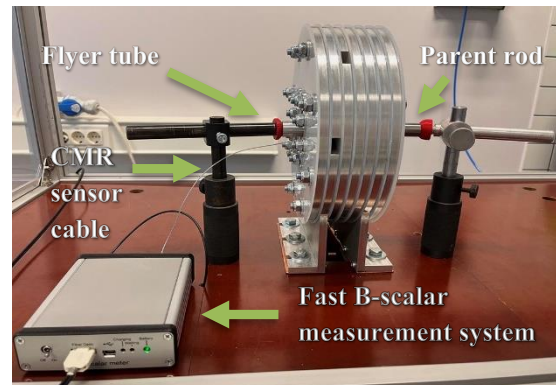


Fig. 1. The work table in the MPW setup contains samples of the flyer tube and the parent rod, which are inserted into the Bitter coil and fast B-scalar measurement system.

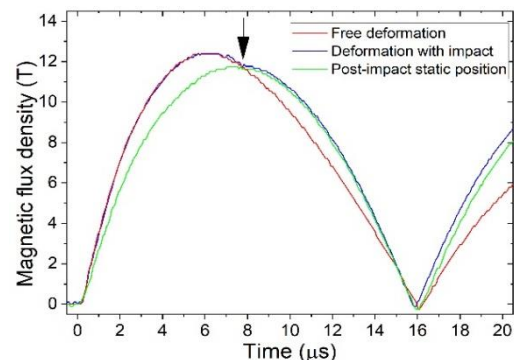


Fig. 2. Time dependence of magnetic flux density during crimping of the flyer tube around steel rod (blue). The arrow shows the moment of impact. Remeasuring of crimped parts (green).

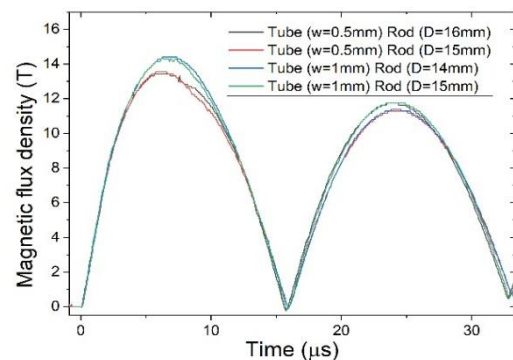


Fig. 3. Time dependence of magnetic flux density during crimping of the flyers around the rods with different geometrical parameters

References

1. Sensors 2020, 20(20), 5925; Doi: 10.3390/s20205925.
2. Sensors 2023, 23(3), 1435; Doi: 10.3390/s23031435.

Development and Characterization of CoFe/Cu-based Spin-Valves

Darius Antonovič¹, Vilius Vertelis¹, Andrius Maneikis¹, Nerija Žurauskienė¹

1. Center for Physical Sciences and Technology, Department of Functional Materials and Electronics
Saulėtekio av. 3, LT-10257 Vilnius, email: darius.antonovic@ftmc.lt

Spin valves are spintronic devices that exhibit giant magnetoresistance (GMR), caused by spin dependent scattering in ferromagnetic materials. The GMR effect itself was simultaneously discovered by both A. Fert's [1] and P. Grünberg's [2] research teams, who observed a significant reduction in the electrical resistance in multilayered Fe/Cr nanostructures when an external magnetic field was applied. These structures were composed of nm thick ferromagnetic Fe layers separated by nm thick non-magnetic Cr layers. The magnetic field changed the antiparallel alignment of the magnetization directions of the ferromagnetic layers relative to each other to a parallel one, which usually has a lower resistance. The size of the GMR effect can be defined by the magnetoresistance ratio (MR):

$$MR = \frac{\Delta R}{R} \cdot 100\% = \frac{R_{AP} - R_P}{R_P} \cdot 100\%, \quad (1)$$

where R_P and R_{AP} are the electrical resistances for parallel and antiparallel alignment, respectively.

Spin-valves, however, are peculiar due to one of their ferromagnetic layers being pinned to an adjacent antiferromagnetic layer via exchange coupling, whereas the magnetization of the other ferromagnetic layer is free to rotate with the applied magnetic field [3]. Even though spin-valves exhibit lower MR values compared to magnetic multilayers, they are more attractive for practical applications due to them requiring only small magnetic fields in order to induce a change in electrical resistance. Additionally, spin-valves can be converted into magnetic tunnel junctions (MTJ) by replacing the non-magnetic conductive spacer layer with a non-magnetic insulator.

GMR-based devices have achieved a wide array of applications due to their low power usage and cost-efficiency. One of the most prominent fields in data storage, where MTJs and spin-valves are used as reading heads in hard disk drives (HDDs) and in magnetic random-access memory (MRAM), which is nonvolatile, durable and consumes little power [4]. Industrial applications include position sensors, current sensors and non-destructive monitoring. Furthermore, GMR-based biosensors have found applications in biomedical diagnosis, food safety, and environmental monitoring.

A major recent development in the field of spintronics has been the discovery of 2D ferromagnetism in 2017 [5], which has created the conditions for the proliferation of Van der Waals (VdW) spin-valves. VdW spin-valves are typically composed of layered 2D materials, such as ferromagnetic Van der Waals crystals combined with other 2D materials like graphene, which are stacked together to form heterostructures. These specific spin-valves are of major interest to us due to the high tunability of their ferromagnetic transition temperature and ultra-compact design.

Our goal, therefore, was to acquire proficiency in spin-valve production and characterization capabilities for further research in fields related to biosensing and VdW spin-valves. This contribution presents magnetoresistance measurements conducted on our fabricated CoFe/Cu-based spin-valves with IrMn antiferromagnetic pinning.

References

1. M. N. Baibich et al., "Giant Magnetoresistance of (001)Fe/(001)Cr Magnetic Superlattices", *Phys Rev Lett*, **61**(21), 2472 (1988)
2. G. Binasch et al., "Enhanced magnetoresistance in layered magnetic structures with antiferromagnetic interlayer exchange", *Phys Rev B*, **39**(7), 4828 (1989)
3. Tsymbal, E. Y., Pettifor D. G., "Perspectives of giant magnetoresistance", *Solid State Physics*, **56**, 113–237 (2001)
4. S. Yang and J. Zhang, "Current Progress of Magnetoresistance Sensors", *Chemosensors*, **9**(8), 211 (2021)
5. C. Gong et al., "Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals", *Nature*, **546**(7657), 265–269 (2017)

LASER INDUCED SINGLE PHOTON EMITTERS IN HEXAGONAL BORON NITRIDE FOR QUANTUM KEY DISTRIBUTION

Ifra Bibi¹, Vakarīs Šilys¹, Viktorija Nargelienė¹, Julius Janušonis¹, Danielis Rutkauskas¹, Edgaras Markauskas¹, Tadas Paulauskas¹

1. Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius, email: ifra.bibi@ftmc.lt

Single photon emitters (SPEs) are widely used for the development of quantum technologies such as quantum key distribution (QKD), quantum sensing, and quantum computing. Secure QKD networks requires scalable SPEs that can operate at room temperature with high stability and brightness. Hexagonal boron nitride (hBN), a layered two-dimensional wide-bandgap material, has emerged as a promising candidate for hosting SPEs due to its chemical stability, wide optical transparency window, and ability to support defect-based single-photon emission.

In this work, we have created SPEs in multilayer hBN at desired locations using ultrashort laser pulses. Single-photon emission properties from atomic defects in hBN are investigated through scanning confocal photoluminescence microscopy, second-order correlation (Hanbury Brown and Twiss) measurements, and lifetime measurements. Under the optimized fabrication and high temperature annealing conditions, we observed that SPEs emit in the visible to near infrared region.

These results address critical needs for practical QKD sources and pave the way for integrated quantum photonic devices.

References

1. Xu, Q., Gao, B., Zhao, L., Lv, G., Yang, J., & Li, X. (2025). Enhanced Performance of Single-Photon Emitter Hosted in Hexagonal Boron Nitride via Two-Photon Excitation. *ACS Photonics*, 12(4), 2178-2186.
2. Gan, L., Zhang, D., Zhang, R., Zhang, Q., Sun, H., Li, Y., & Ning, C. Z. (2022). Large-scale, high-yield laser fabrication of bright and pure single-photon emitters at room temperature in hexagonal boron nitride. *ACS nano*, 16(9), 14254-14261.

CARRIER DYNAMICS IN n- AND p-TYPE InGaN LAYERS

Seda Türkcan

Vilnius University, Department of Photonics and Nanotechnology
Saulėtekio av. 3, LT-10257 Vilnius, email: seda.turkcan@ff.stud.vu.lt

Indium gallium nitride (InGaN) thin films serve as key materials in modern optoelectronic devices such as light-emitting diodes (LEDs) and laser diodes. The performance of these devices critically depends on the successful integration of both n-type and p-type layers to form high-quality p–n junctions. While n-type conductivity can be achieved through donor doping with elements such as silicon or oxygen, realizing stable and efficient p-type InGaN remains a significant challenge. In this study, we investigate the non-equilibrium carrier dynamics of both n-type and p-type InGaN thin films using Light-Induced Transient Grating (LITG) and Time-Integrated Photoluminescence (TIPL) spectroscopy.

By analyzing carrier lifetime, diffusivity, and diffusion length, we establish their relationship with internal quantum efficiency, allowing a comparative assessment of the two doping regimes. Our findings indicate that a distinct fast-decaying component, absent in n-type samples, is present in the transient decay of p-type samples and does not contribute to carrier diffusion.

DIRECTLY GROWN GRAPHENE ON ANNEALED AND NON-ANNEALED SiO₂ FILMS OF DIFFERENT THICKNESSES

Muhammad Adnan Saeed¹, Šarūnas Meškinis¹, Rimantas Gudaitis¹, Asta Guobienė¹

1. Institute of Materials Science, Kaunas University of Technology, K. Baršausko g. 59, LT-51423, Kaunas

email: Muhammad.saeed@ktu.edu

Graphene, with its exceptional electrical, mechanical, and biocompatible properties, has emerged as a promising material for biosensing applications. However, conventional graphene synthesis methods often involve complex transfer processes that introduce defects and impurities, limiting device performance. This study explores the direct growth of graphene using Plasma-Enhanced Chemical Vapor Deposition (PECVD) on desired substrates, eliminating the need for transfer and preserving graphene's intrinsic properties. PECVD enables the low-temperature, catalyst-free synthesis of graphene directly on various dielectric and polymer substrates.[1] This method not only preserves substrate integrity but also enhances the integration potential for flexible and wearable biosensing platforms. Our research successfully synthesizes high-quality monolayer and few-layer graphene films with tunable properties by optimizing plasma power, precursor flow rates, and substrate temperatures on annealed and non-annealed SiO₂ films of 100nm and 300nm thickness. Raman spectroscopy, SEM, and electrical measurements confirm the structural integrity and conductivity of the graphene films. The direct PECVD-grown graphene platform holds significant potential for next-generation biosensors, enabling real-time, label-free detection with improved stability and performance. Direct PECVD-grown graphene biosensors for COVID detection could revolutionize point-of-care testing, enabling real-time monitoring and early outbreak containment. This work highlights the potential of advanced nanomaterials in combating global health crises through innovative sensing solutions.

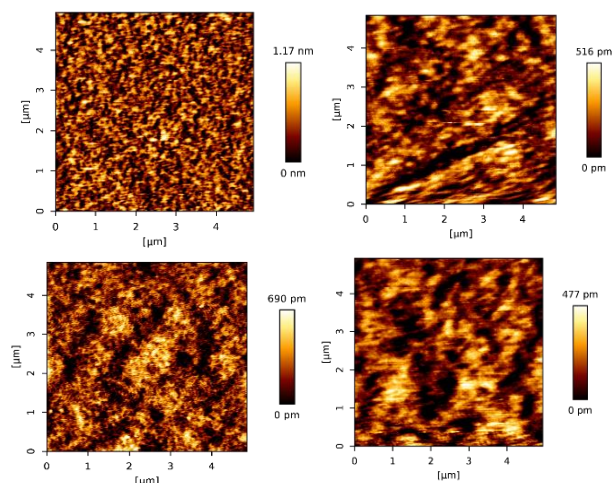


Fig 1: AFM images of a) Graphene on 100nm annealed SiO₂, b) Graphene on 100nm non-annealed SiO₂ c) Graphene on 300nm annealed SiO₂, d) Graphene on 300nm non-annealed SiO₂

The process of Microwave plasma-enhanced chemical vapor deposition works by using methane gas as the source of carbon, and hydrogen gas is used for the etching of carbon. A Si (100) wafer coated with 300 nm and 100 nm thick silicon dioxide (SiO₂) films was used as the substrate. PECVD introduces a plasma, which provides reactive radicals and ions, lowering the activation energy for carbon precursor decomposition.[2]

References:

1. Li, M., Liu, D., Wei, D., Song, X., Wei, D., & Wee, A. T. S. (2016). Controllable synthesis of graphene by plasma-enhanced chemical vapor deposition and its related applications. *Advanced Science*, 3(11), 1600003.
2. Meškinis, Š., Vasilaiuskas, A., Guobienė, A., Talaikis, M., Niaura, G., & Gudaitis, R. (2022). The direct growth of planar and vertical graphene on Si (100) via microwave plasma chemical vapor deposition: synthesis conditions effects. *RSC advances*, 12(29), 18759-18772.

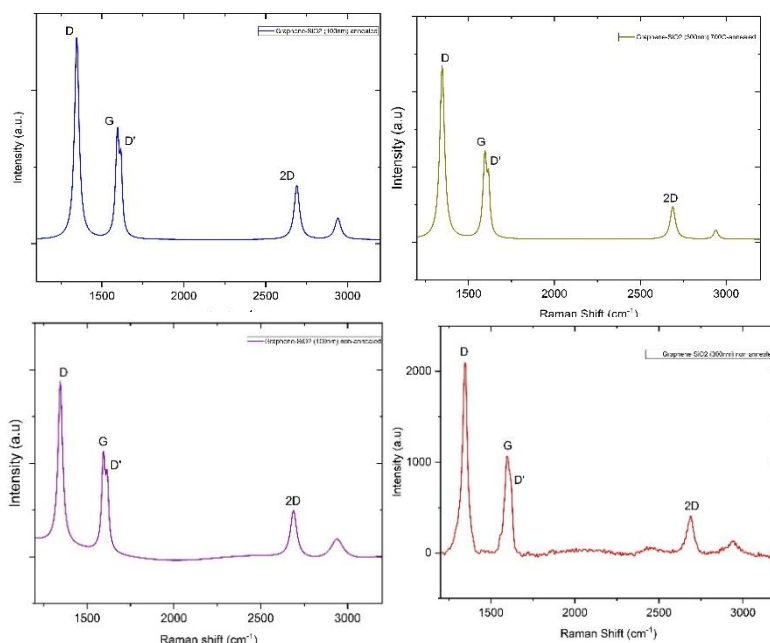


Fig 2: Raman Spectra of Graphene on 100nm and 300nm SiO₂ substrate, annealed and non-annealed.

Extending Bismide Emitter Applications from Medicine to Telecommunication

Aivaras Špokas¹, Andrea Zelioli¹, Mindaugas Kamarauskas², Virginijus Bukauskas², Bronislovas Čechavičius¹, Andrius Bičiūnas¹, Evelina Dudutienė¹, Renata Butkutė¹.

¹Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius, email: aivaras.spokas@ftmc.lt

²Center for Physical Sciences and Technology, Department of Physical Technology
Saulėtekio av. 3, LT-10257 Vilnius

Near-infrared (NIR) is a widely used emission region for applications in a plethora of fields due to its advantageous properties. Medical applications benefit from a large penetration depth into human tissue, enabling sensors of vital parameters and therapeutics. Negligible losses and dispersion of NIR emission in fiber optics are essential for telecommunications. Finally, applications in environmental monitoring, like pollution sensors or LiDAR, benefit from the atmospheric transparency, eye-safety, and a well-developed detector market. Even though the mentioned applications fall in the same NIR region, they require inherently different parameters to work effectively. Semiconductor emitters, like light-emitting and laser diodes, allow varying the device parameters by adapting the technological processes of device fabrication to suit a certain wavelength and power. One way to achieve a variation in device parameters is to utilize material engineering to cater to different application needs. NIR has two main semiconductor wafer platforms: (i) InP is used for the longer emission wavelengths, since it is possible to produce emitters for telecom C-band by growing lattice-matched InGaAs; (ii) GaAs platform is mainly used for wavelengths up to 1 μm , where managing the strain in mismatched GaAs/InGaAs quantum structure is not difficult. A problematic range of emission wavelength is between the two mentioned material systems since the lattice mismatch becomes a crucial issue, preventing the production of high-efficiency devices. We propose bismides as a solution for emissions above 1 μm up to the telecom O-band, starting at 1260 nm. The appeal of introducing Bi into the GaAs lattice stems from its attractive properties in the NIR emission range. First, the introduction of Bi results in a rapid bandgap narrowing of up to 88 meV/%Bi, which is beneficial in avoiding lattice mismatch dislocations, since a low concentration of Bi shifts the wavelength substantially [1]. Furthermore, the success of bismides could tackle two of the major efficiency bottlenecks of narrow bandgap emitters, both in suppressing Auger recombination and enabling stable room-temperature operation without the need for cooling systems, resulting in better wall-plug efficiency [2, 3]. Furthermore, such emitters are spectrally stable in a wide temperature range.

In this work, we demonstrate the capabilities of producing application-focused NIR devices in the biomedical window for possible applications in enhanced accuracy blood oxygen sensors [4]. Additionally, a future perspective of the investigated alloys is shown by growing quantum structures emitting in the telecom O-band wavelength region,

demonstrating their potential as an active medium for subsequent application in devices. The structures presented in the work were grown using a Veeco GENxplor R&D molecular beam epitaxy system, which enabled the growth of device structures with high precision and advanced designs such as parabolically graded barriers. The fabricated devices utilized a similar layer structure with the doped AlGaAs layers sandwiching a GaAsBi/GaAs rectangular quantum well (RQW) active area. The produced LEDs were shown to cover an emission region of around 1000 to 1200 nm. While the laser diodes had central emission peaks at 1000, 1030, and 1140 nm. An RQW laser diode was capable of 10 mW of peak power, though it had a large threshold current above 2 A. Utilizing parabolically graded barriers, the threshold current was decreased by an order of magnitude, and the maximum output power of 140 mW was registered. Despite these improvements, due to the defects induced by the low-temperature growth of GaAsBi, the structures were lasing only under pulsed electrical excitation. Additionally, some device structures were grown on AlAs sacrificial layers that can be etched out to remove the native substrates. Such structures are prepared for integrated photonic circuits, where the components can be transferred using flip-chip bonding. Thus, the structures must be grown using a non-standard flipped configuration, resulting in technological challenges. A decreased substrate temperature was used to achieve an acceptable dopant distribution in the structure, demonstrating the technological capability of growing integration-ready devices. Finally, investigations continued on growing quantum structures capable of emission in the longer wavelength regions. A GaAsBi RQW structure exhibited room temperature photoluminescence (PL) at a central wavelength of 1325 nm, while the use of a quaternary alloy InGaAsBi allowed achieving a more intense PL spectrum while maintaining a long emission wavelength of 1265 nm.

References

1. S. Francoeur et al., Appl. Phys. Lett. 82 (22), 3874–3876 (2003)
2. Y. Tominaga et al., Appl. Phys. Exp. 3 (6) (2010)
3. K. Alberi et al., Appl. Phys. Lett. 91 (5), 10–13 (2007)
4. A. Špokas et al., Micromachines 16(5), 506 (2025)

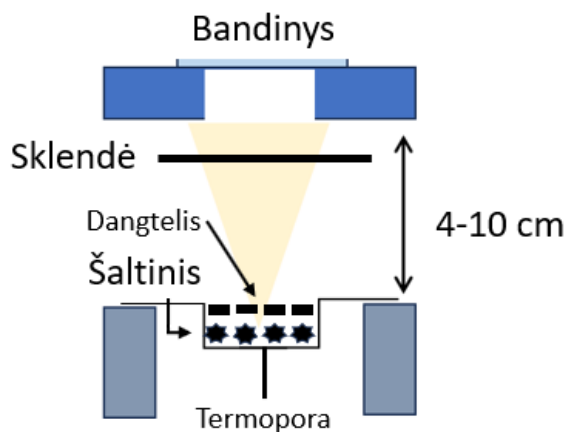
SbSel dangų nusodinimo optimizavimas terminio garinimo metodu

Deividas Vainauskas¹, Vidas Pakštas¹, Rokas Kondrotas¹

1. Fizinių ir technologijos mokslų centras, Medžiagų struktūrinės analizės skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: deividas.vainauskas@ftmc.lt

Stibio seleno jodidas (SbSel) trinaris junginys, kuris kelia vis didesnę susidomėjimą fotovoltaiškos srityje. Dėl savo didelio šviesos sugerties koeficiento regimojoje srityje bei plataus draustinės juostos tarpo (1,7-2,0 eV), jis turi didelį potencialą kuriant naujos kartos fotovoltinius elementus sugeriant vidaus patalpų (*angl.* indoor photovoltaics) apšvietimą. Ši medžiaga sudaryta iš nebrangių ir mažai toksiškų elementų ir yra termodinamiškai stabili kambario temperatūroje [1]. Tačiau SbSel kristalinę struktūrą sudaro gijos, kurios pagrindine kryptimi sudariusios stiprius kovalentinius ryšius, o kitomis – van der Valsinius. Taigi medžiagai kristalizuojantis susidaro adatėlių formos primenantį grūdėlių struktūrą. Tokia morfologija nėra tinkama daugiasluoksniams saulės elementams nes lemia padidintą paviršinę rekombinaciją ir dėl neužtikrinamo dangos vientisumo – mažą kontaktinį plotą. Taigi, pagrindinis darbo tikslas nustatyti optimalias terminio garinimo sąlygas norint suformuoti kompaktiškas, lygias ir stochiometrinės SbSel dangas.

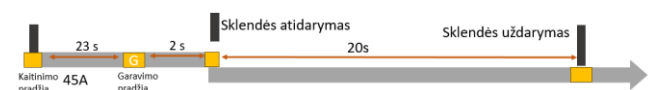
Šiame darbe buvo naudojama terminio užgarinimo metodika gauti SbSel sluoksnius ir buvo keičiami šie parametrai: atstumas tarp šaltinio ir bandinio (4 – 10 cm); sklendės užsidarymo atsidarymo laikai, tiek garinimo pradžioje, tiek pabaigoje; per lovėlių tenkančios srovės dydis (40-73 A); lovėlių dangtelių formos (pav. 1).



1 pav. Principinė terminio garinimo sistemos schema.

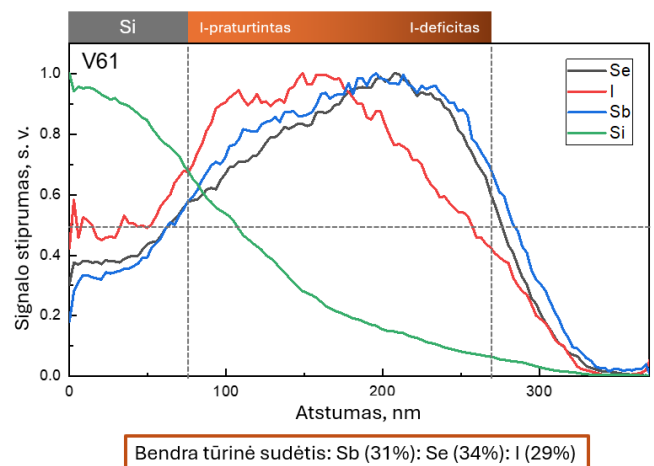
Nustatyta, kad keičiant bandinio aukštį, ypač kinta dangos storis, pasirinktas geriausias aukštis 5 cm, siekiant gauti ~300 nm dangas garinant iš 20 mg medžiagos.

Keičiant sklendės atidarymo/uždarymo laikus, nustatytas optimalus garinimo režimas pavaizduotas 2-ame paveiksle. Prie šių sąlygų yra gaunamas geriausias Sb, Se ir I elementų pasiskirstymas tūryje (pav. 3) ir elementų santykis artimas 1:1:1.



2 pav. Optimalios sąlygos siekiant gauti stochiometrinę SbSel dangą, esant 45 A kaitinimo srovės stipriui.

Tyrimai parodė, kad net ir prie didelių kaitinimo greičių (>4 °C/s), SbSel skilimo reakcijos nebuvo galima išvengti. Todėl panaudojant sklendę tiek garavimo pradžioje, tiek pabaigoje buvo sumažinta skilimo produktų įtaka dangos sudėčiai ir gauta norimos stochiometrijos SbSel pirmtako danga.



3 pav. Sb, Se ir I elementų pasiskirstymas SbSel dangoje užgarintoje optimaliomis sąlygomis.

Literatūra:

1. Sadurni, Marc Dolcet, et al. "Preparation and characterization of SbSel thin films." *Journal of Science: Advanced Materials and Devices* 9.1 (2024): 100664.
2. Nowak, M., et al. "Optical properties of nanocomposite fibrous polymer mats containing SbSel nanowires." *Optical Materials* 84 (2018): 383-388.

Surface-Modified MXenes as Promising Adsorbents for Organic Pollutant Elimination

Germantė Paulikaitė¹, Aswathi Raveendran¹, Agnė Sukovienė, Arūnas Jagminas¹, Simonas Ramanavičius¹

1. Center for Physical Sciences and Technology, Department of Electrochemical Material Science, nanostructure laboratory

Saulėtekio av. 3, LT-10257 Vilnius, email: germante.paulikaite@ftmc.lt

MXenes, a novel two-dimensional nanomaterial class, discovered in 2011 at Drexler University, have already gained huge scientific attention due to their unique properties such as plasmonic behavior, hydrophilicity, and outstanding electrical and mechanical performance [1]. The number of publications regarding MXenes' potential applications across various fields is rapidly increasing since these structures are easier to functionalize and synthesize demonstrating versatility over other 2D materials e.g. graphene.

While the synthesis process is relatively straightforward usually involving selective transition metal etching by using strong acids. This treatment results in sheet-like layered structures, which can be further delaminated into thinner flakes, dramatically increasing surface area and enhancing their reactivity. The most studied MXene structure among many others is Ti₃C₂T_x, which was also employed in this study.

MXenes continuously attract research of interest because of tunable surface chemistry, adsorption, and high electrical conductivity. Nowadays MXenes are successfully employed in Raman spectroscopy [2], biofuel elements [3], lithium and sodium ion batteries [4]. Moreover, MXenes have demonstrated potential in catalysis, energy storage devices (supercapacitors, lithium/sodium-ion batteries), biofuel cells, biosensing, and drug delivery systems.

Emerging organic dye pollution coming from the textile and painting industries caused environmental concerns due to its toxicity to humans and raising biodegradation resistance. Therefore, adsorption-based technologies offer a cost-effective and efficient alternative. Fortunately, the favorable large surface area, tunable surface chemistry of MXenes provides strong platform for removing such contaminants

In this study, delaminated and differently functionalized MXene structures were investigated for the removal of organic dyes in aqueous solutions. Specifically, Methylene Blue, Azure A, and Rhodamine B dyes were chosen due to their widespread usage in the textile industry. Distinct adsorption interactions were observed for both types of MXene structures. For better adsorption evaluation adsorption capacities Q , (g/g) were calculated to compare dye removal efficiency and the influence of different surface termination groups.

Acknowledgment: This project received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-24-14.

References

1. Gogotsi Y, Anasori B. The Rise of MXenes. *ACS Nano* 2019; 13:8491–4. <https://doi.org/10.1021/acsnano.9b06394>.
2. Adomavičiūtė-Grabusovė S, Ramanavičius S, Popov A, Šablinskis V, Gogotsi O, Ramanavičius A. Selective enhancement of SERS spectral bands of salicylic acid adsorbate on 2D Ti₃C₂T_x-based MXene film. *Chemosensors* 2021; 9:223.
3. Ramanavicius S, Ramanavicius A. Progress and Insights in the Application of MXenes as New 2D Nano-Materials Suitable for Biosensors and Biofuel Cell Design. *Int J Mol Sci* 2020;21. <https://doi.org/10.3390/ijms21239224>.
4. Li X, Huang Z, Shuck CE, Liang G, Gogotsi Y, Zhi C. MXene chemistry, electrochemistry and energy storage applications. *Nat Rev Chem* 2022; 6:389 404.

BIMETALINĖS NANOSTRUKTŪROS SUSTIPRINTO RAMANO SKLAIDOS TYRIMAMS

Gytautė Sirgėdaitė¹, Martynas Talaikis¹, Shivani Yadav², Vladimir Sivakov², Lina Mikoliūnaitė¹

1. Fizinių ir technologijos mokslų centras, Organinės chemijos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: gytaute.sirgedaite@ftmc.lt
2. Leibnico fotoninių technologijų institutas, Albert-Einstein g. 9, 07745, Jena, Vokietija

Paviršiaus sustiprinta Ramano spektroskopija (SERS) yra pažangi analizės technika, taikoma tiksliniam molekulių struktūros identifikavimui ir charakterizavimui. Šis metodas išsiskiria dideliu jautrumu ir selektyvumu, todėl gali būti naudojamas įvairiose srityse – nuo cheminių junginių analizės iki biologinių medžiagų aptikimo. SERS signalo sustiprinimas pasiekiamas naudojant nanostruktūrinius plazmoninius metalus, tokius kaip auksas (Au), sidabras (Ag) ir varis (Cu) [1]. Pastaraisiais metais buvo sukurta įvairių nanostruktūrinių substratų – nanodalelių, strypų, žvaigždžių formos darinių ir dendritų, dažniausiai sudarytų iš Ag, Au arba Cu. Šiuo struktūrų projektavimu ir sinteze siekiama optimizuoti plazmonines savybes bei padidinti SERS aktyvumą. Vis daugiau dėmesio skiriama bimetalinėms nanostruktūroms, kurios pasižymi unikalėmis savybėmis, kurių negalima pasiekti monometalinėse sistemose. Tokios struktūros, kaip bimetalinės šerdies–apvalkalo nanodalelės ar bimetaliniai dendritai, demonstruoja padidintą SERS efektyvumą, palyginti su jų monometaliniais analogais [2]. Nanodalelių dydžio, formos ir aplinkos optimizavimas yra esminis veiksnys, lemiantis plazmoninį jautrumą molekuliniam bei biologiniam nustatymui. Sustiprintas artimasis elektromagnetinis laukas sudaro prielaidas formuoti SERS substratus, pasižyminčius dideliu stiprinimo koeficientu ir karštųjų taškų (hot spots) tankiu. Tokie substratai leidžia kurti itin jautrius aptikimo metodus [3].

Šiame darbe pristatomos Au–Ag šerdies–apvalkalo bimetalinės nanodalelės ir Cu–Ag dendritinės nanostruktūros, formuotos ant silicio (Si) plokštelės paviršiaus. Aukso šerdies nanodalelės buvo susintetintos ir, reguliuojant AgNO_3 koncentraciją, padengtos įvairaus storio sidabro apvalkalais. Stabilumo tyrimai parodė, kad plonesni sidabro apvalkalai pagerina atsparumą oksidacijai ir agregacijai, o storesni sluoksniai padidina SERS aktyvumą. Ergotioneino – biologiškai svarbaus antioksidanto ir potencialaus vėžio biožymens – tyrimai parodė, kad naudojant Au–Ag šerdies–apvalkalo bimetalines nanostruktūras galima pasiekti 10^{-6} M aptikimo ribą, atitinkančią fiziologinę koncentraciją kraujo serume.

Tuo tarpu Cu–Ag dendritinės struktūros buvo nusodintos ant silicio pagrindo elektrocheminės redukcijos būdu, naudojant galvaninio pakeitimo reakciją. Kaip sidabro šaltiniai naudotos trys skirtingos druskos – AgNO_3 , Ag_2SO_4 , Ag_3PO_4 . Keičiant Cu:Ag tūrio santykius, buvo gautos struktūros, pasižyminčios skirtingomis morfologinėmis savybėmis. Šios nanostruktūros buvo pritaikytos SERS taikymams plačiame sužadinimo diapazone – nuo UV iki artimojo infraraudonojo (IR). Ypatingai svarbu pažymėti, kad SERS signalo sustiprėjimas buvo stebėtas UV diapazone ant Cu pagrindo paviršių – šis efektas iki šiol literatūroje nebuvo aprašytas [4]. Siekiant dar labiau išplėsti SERS aktyvumą artimojo IR srityje, į sistemą buvo įtrauktas sidabras, kuris užtikrino efektyvesnį plazmoninį atsaką.

Literatūra

1. L. Liu, T. Gao, Q. Zhao, Z. Xue, and Y. Wu, Opt. Laser Technol. 181, 111827 (2025).
2. K. Chang and H. Chung, RSC Adv. 6(79), 75943–75950 (2016).
3. J. Katyal, Rev. Plasmonics 2017, 77–108 (2019).
4. S. Yadav, M. Talaikis, Y. V. Ryabchikov, M. Ziegler, G. Niaura, T. Deckert-Gaudig, and V. Sivakov, Adv. Opt. Mater. 13(18), 2500078 (2025).

Azotu ir metalais legiruotos biomasinės anglies katalizatorių (AWC-Co-N, AWC-Cu-N) sintezė ir jų taikymas hidrazino oksidacijai

Virginija Ulevičienė¹, Loreta Tamašauskaitė Tamašiūnaitė¹

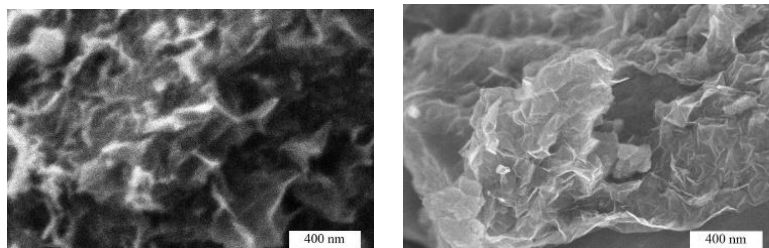
1. Fizinių ir technologijos mokslų centras, Katalizės skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: virginija.uleviciene@ftmc.lt

Augantis poreikis tvariems ir efektyviems energijos konversijos sprendimams skatina ieškoti pigių, aplinkai draugiškų ir aukštą aktyvumą turinčių katalizatorių. Šiame tyrime buvo sukurti katalizatoriai, pagaminti panaudojant iš biomasės gautą aktyvintą anglį (AWC) ir modifikuoti kobalto-azoto (AWC-Co-N) bei vario-azoto (AWC-Cu-N) deriniais. Medžiagos buvo gautos vieno žingsnio terminiu būdu, naudojant dicianidamidą (DCDA) kaip azoto šaltinį ir Co^{2+} arba Cu^{2+} jonus kaip dopantus. Po pirolizės, atliktos 800 °C temperatūroje, katalizatoriai buvo išsamiai charakterizuoti taikant ICP-OES, XRD, XPS, SEM-EDS, BET paviršiaus analizę ir Ramano spektroskopiją.

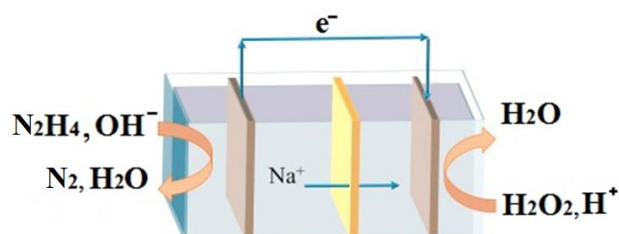
Elementinė analizė parodė, kad AWC-Co-N sudėtyje yra ~1,29 at.% Co ir 98,71 at.% C, o AWC-Cu-N – ~1,19 at.% Cu ir 98,81 at.% C. Abiejų katalizatorių elektrokatalitinės savybės buvo tirtos atliekant hidrazino (N_2H_4) elektrocheminę oksidaciją 1 M KOH tirpale naudojant ciklinę voltamperometriją. Tyrimai atskleidė, kad tiek AWC-Co-N, tiek AWC-Cu-N pasižymi aukštu elektrokatalitiniu aktyvumu ir stabilumu, o tai liudija jų potencialą kaip efektyvių anodinių medžiagų tiesioginiuose hidrazino kuro elementuose (DHFC). Papildomai, katalizatoriai buvo išbandyti tiesioginio $\text{N}_2\text{H}_4\text{--H}_2\text{O}_2$ kuro elemento prototipe, naudojant juos tiek anodo, tiek katodo medžiagomis. Anolitu buvo naudojamas 1 M N_2H_4 + 1 M KOH tirpalas, o kaip katolitas – 5 M H_2O_2 + 1,5 M HCl. Anolitą nuo katolito skyrė Nafion®117 membrana. Eksperimentai parodė, kad abu katalizatoriai pasižymi aukštu aktyvumu ir geru stabilumu, todėl yra tinkami naudoti kaip elektrodo medžiagos tvariose kuro elementų sistemose.

Tyrimo rezultatai rodo, kad azotu ir pereinamaisiais metalais legiruota anglis, gauta iš biomasės, yra perspektyvi platforma nebrangiems, netauriųjų metalų pagrindu sukurtiems elektrokatalizatoriams, galintiems pakeisti tauriuosius metalus tiek kuro elementuose, tiek kituose elektrocheminiuose įrenginiuose.

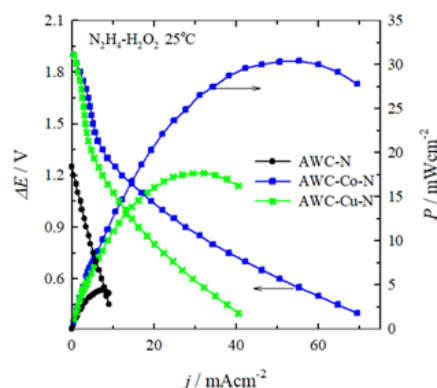
Be to, šie rezultatai pabrėžia tokių medžiagų potencialą tvariai elektrokatalizei, ypač technologijose, kurios siekia suderinti našumą, aplinkosaugą ir mažas sąnaudas.



1 pav. SEM vaizdai AWC-Co-N (a) ir AWC-Cu-N (b) katalizatorių.



2 pav. Tiesioginio $\text{N}_2\text{H}_4\text{--H}_2\text{O}_2$ kuro elemento veikimo schema.



3 pav. Celės poliarizacijos ir galios tankio kreivės tiesioginiame $\text{N}_2\text{H}_4\text{--H}_2\text{O}_2$ kuro elemente, naudojant AWC-N, AWC-Co-N ir AWC-Cu-N katalizatorius. Anolitas – 1 M N_2H_4 + 1 M KOH, katolitas – 5 M H_2O_2 + 1,5 M HCl.

Cobalt-Based Electrocatalysts: A Pathway Toward Cost-Effective and High-Performance Water Splitting

Huma Amber¹, Aldona Balčiūnaitė¹, Zita Sukackienė¹, Loreta Tamasauskaite-Tamasiunaite¹, Eugenijus Norkus¹

1. Center for Physical Sciences and Technology, Department of Catalysis
Saulėtekio av. 3, LT-10257 Vilnius, email: huma.amber@ftmc.lt

The production of green hydrogen through water splitting is considered to be one of the most environmentally friendly and practical solutions to address the global energy crisis and mitigate the greenhouse effect. A primary challenge in the field concerns the development of efficient, stable, and cost-effective electrocatalysts capable of facilitating both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER), particularly in alkaline media. Transition metal phosphides (TMPs) are recognised as electrocatalysts of significant effectiveness. In this study, cobalt-phosphorus (CoP) coatings with varying phosphorus contents (0.4, 1.6, 5, 8, and 11 wt% P), cobalt-iron-phosphorus (CoFeP), and their palladium-modified derivatives (PdCoP and PdCoFeP) were engineered on copper substrates via a facile electroless deposition process followed by Pd incorporation through the galvanic displacement method. While other noble metals, including platinum (Pt) and rhodium (Rh), are frequently employed in catalytic applications due to their superior catalytic efficiency, palladium (Pd) was selected for this study due to its distinctive equilibrium of catalytic performance and comparatively reduced cost. Sodium hypophosphite (NaH_2PO_2) was utilized as the reducing agent. The morphology, structure, and composition of

the coatings were analyzed using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX), and their electrocatalytic activities for the HER, OER, and overall water splitting (OWS) were evaluated in 1 M KOH.

The investigation revealed a strong correlation between the activity of CoP coatings and the phosphorus content. For the HER, $\text{CoP}_{11}/\text{Cu}$ demonstrated optimal performance with an overpotential of 98.9 mV at 10 mA cm^{-2} , while for the OER, CoP_8/Cu exhibited the lowest overpotential of 378 mV at 10 mA cm^{-2} . Palladium modification has been demonstrated to substantially enhance catalytic kinetics and stability. An electrolyzer composed of PdCoFeP as both the anode and cathode has been shown to exhibit an OWS cell voltage of 1.69 V at 10 mA cm^{-2} in 1 M KOH. This result is particularly noteworthy when compared to other electrodes, such as PdCoP/Cu (1.78 V) and $\text{CoP}_{11}/\text{Cu}$ (1.81 V). The findings of this study demonstrate that compositional tuning of CoP and CoFeP coatings, in conjunction with Pd deposition via galvanic displacement, effectively enhances the bifunctional catalytic performance of the coatings. This finding indicates that this combination of processes may offer a promising route for cost-effective and sustainable hydrogen generation.

NIKELIO-KOBALTO DANGŲ CHEMINIS NUSODINIMAS IR TAIKYMAS VANDENILIO GENERAVIMUI / CHEMICAL DEPOSITION OF NICKEL-COBALT COATINGS AND APPLICATION FOR HYDROGEN GENERATION

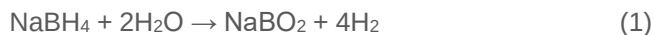
Gitana Valeckytė¹, Zita Sukackienė¹, Virginija Kapenienė¹, Jūratė Vaičiūnienė¹, Loreta Tamašauskaitė
Tamašiūnaitė¹ ir Eugenijus Norkus¹

1. Fizinių ir technologijos mokslų centras, Katalizės skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: gitana.valeckyte@ftmc.lt

Išseikvojamos iškastinio kuro atsargos, nuolatinė aplinkos tarša ir visuotinis atšilimas, tai yra trys didžiausios šių laikų problemos. Pastarąjį lemia anglies dioksido ir kitų dujų kiekio padidėjimas. Visi šie veiksniai paskatino vandenilio, kaip vieno perspektyviausių ateities energijos šaltinių, paieškas ir tyrimus [1].

Vandenilis gali būti išgaunamas iš įvairių medžiagų, tokių kaip vanduo (H_2O), metalų hidridai ($NaBH_4$, KBH_4 , $LiBH_4$, $NaAlH_4$, MgH_4), hidrazino hidratai ($N_2H_4 \cdot H_2O$), hidrazinas arba amonio boranai ($N_2H_4 \cdot BH_3$, $NH_4 \cdot BH_3$), skruzdžių rūgštis ($HCOOH$), metanolis (CH_4O). Viena svarbiausių vandenilio kaupimo medžiagų savybių yra didelė jų gravimetrinė vandenilio talpa.

Didžiausią vandenilio talpą turi šios medžiagos: $N_2H_4BH_3$ (15,4 masės %), $LiBH_4$ (18,5 masės %), $Mg(BH_4)_2$ (14,9 masės %), NH_3BH_3 (19,6 masės %), NH_3 (17,7 masės %), $NaBH_4$ (10,8 masės %) ir $N_2H_4 \cdot H_2O$ (8 masės %). Dėl to šios medžiagos laikomos perspektyviomis vandenilio kaupimui ir naudojimui nešiojamuose kuro elementuose [2]. Natrio borohidridas ($NaBH_4$) išsiskiria iš kitų hidridų keliomis vertingomis savybėmis: jis yra pigus, nedegus, ekologiškas, stabilus šarminiuose tirpaluose, atsinaujinantis (t. y. gali būti regeneruojamas iš natrio borato), netoksiškas ir nereikalaujantis specialių laikymo ar veikimo sąlygų [3]. Šis junginys priklauso koordinacinio tipo hidridams. Jo katijonai yra metalo jonai, turintys didelį potencialą vandenilio gamybai, nes 1 molis $NaBH_4$ gali būti hidrolizuojamas, išskiriant 4 molius H_2 dujų. Vandenilio išsiskyrimą iš natrio borohidrido galima apibūdinti šia reakcijos lygtimi [4]:



Nors natrio borohidrido savaiminė hidrolizė kambario temperatūroje vyksta gana lėtai, ją galima visiškai slopinti esant stipriai šarminėms sąlygoms [1]. Dėl to efektyvi natrio borohidrido hidrolizė įmanoma tik esant tinkamam katalizatoriui.

Šio darbo tikslas buvo suformuoti $Ni_{96}Co_4/Cu$, $Ni_{90}Co_{10}/Cu$, $Ni_{80}Co_{20}/Cu$, $Ni_{20}Co_{80}/Cu$ ir $Ni_{10}Co_{90}/Cu$ katalizatorius, juos charakterizuoti ir įvertinti jų katalizines savybes natrio borohidrido hidrolizės reakcijai. Visos NiCo dangos buvo nusodintos ant Cu pagrindo paprastu cheminiu nusodinimo metodu, naudojant morfolino boraną kaip reduktorių. Buvo gauti katalizatoriai su skirtingu kobalto masės procentiniu kiekiu: 4, 10, 20, 80 ir 90. Katalizatorių paviršiaus morfologija, struktūra ir cheminė sudėtis buvo ištirta naudojant skenuojančią elektronų mikroskopiją (SEM) ir indukuotos plazmos optinės emisijos spektroskopiją (ICP-OES), Rentgeno spindulių fotoelektronų

spektroskopiją (XPS), Rentgeno spindulių difrakcijos spektroskopiją (XRD) ir Rentgeno spindulių energijos dispersinę analizę (EDS). Natrio borohidrido hidrolizės reakcijos katalizinis aktyvumas buvo įvertintas išmatuojant vandenilio kiekį, išsiskiriantį iš katalizuojamos natrio borohidrido hidrolizės reakcijos. Darbo metu buvo suformuoti visi minėti NiCo/Cu katalizatoriai. Buvo ištirta jų morfologija ir struktūra. Nustatyta, kad paruoštos dangos susideda iš įvairaus dydžio dalelių, kurios susijungia į ovalo formos aglomeratus. Jų vidutinis dydis siekia nuo 0,1 iki 2,5 μm . Taip pat visos tirtos dangos yra kompaktiškos, be jokių įtrūkimų ar defektų ir pasižymėjo kataliziniu aktyvumu natrio borohidrido hidrolizės reakcijai. Nustatyta, kad dviejų komponentų $Ni_{10}Co_{90}$ danga pasižymėjo didžiausiu kataliziniu aktyvumu. Nustatyta, kad vandenilio išsiskyrimo greitis priklauso nuo kobalto kiekio katalizatoriuose ir darbinio tirpalo temperatūros. Kuo didesnis kobalto kiekis yra katalizatoriuose ir kuo didesnė darbinio tirpalo temperatūra, tuo vandenilio išsiskyrimo greitis yra didesnis. Vandenilio išsiskyrimo greitis nuo 5,09 iki 15,61 ml/min buvo pasiektas esant 343 K temperatūrai, naudojant NiCo/Cu katalizatorius su įvairiu kobalto kiekiu, atitinkamai nuo 4 iki 90 masės %.

1 lentelė. Nusodintų Ni ir Co įkrova visuose suformuotuose katalizatoriuose, nustatyta indukuotos plazmos optinės emisijos spektroskopijos (ICP-OES) metodu.

Katalizatorius	Elementas, masės%		Elementas, $\mu g\ cm^{-2}$		
	Ni	Co	Ni	Co	Ni + Co
$Ni_{96}Co_4/Cu$	96,4	3,6	1047,0	38,5	1085,5
$Ni_{90}Co_{10}/Cu$	89,9	10,1	789,0	88,2	877,2
$Ni_{80}Co_{20}/Cu$	79,6	20,4	732,9	188,1	921,0
$Ni_{20}Co_{80}/Cu$	22,6	77,4	179,4	614,0	793,4
$Ni_{10}Co_{90}/Cu$	9,6	90,4	52,5	496,3	548,8

Literatūra

1. M. Rakap; E. E. Kalu; S. Ozkar. Journal of Alloys and Compounds. 509, 7016-7021 (2011).
2. Q. Yao; Y. Ding; Z. H. Lu. Inorg. Chem. Front. 7, 3837 (2020).
3. A. Ekinici; N. Genli; O. Sahin; O. Baytar. Int. J. of Hydrogen Energy. 51, 796-808 (2024).
4. Y. Guo; Z. Dong; Z. Cui; X. Zhang; J. Ma. Int. J. of Hydrogen Energy. 37, 1577-1583 (2012).

Development of Electron Deficient Phosphine Ligands for Palladium(II) Catalysed Fluorination of Arenes

Tomas Paškevičius¹, Ringailė Lapinskaitė¹, Romualdas Striela¹, Jonas Paukštys¹, Linas Labanauskas¹

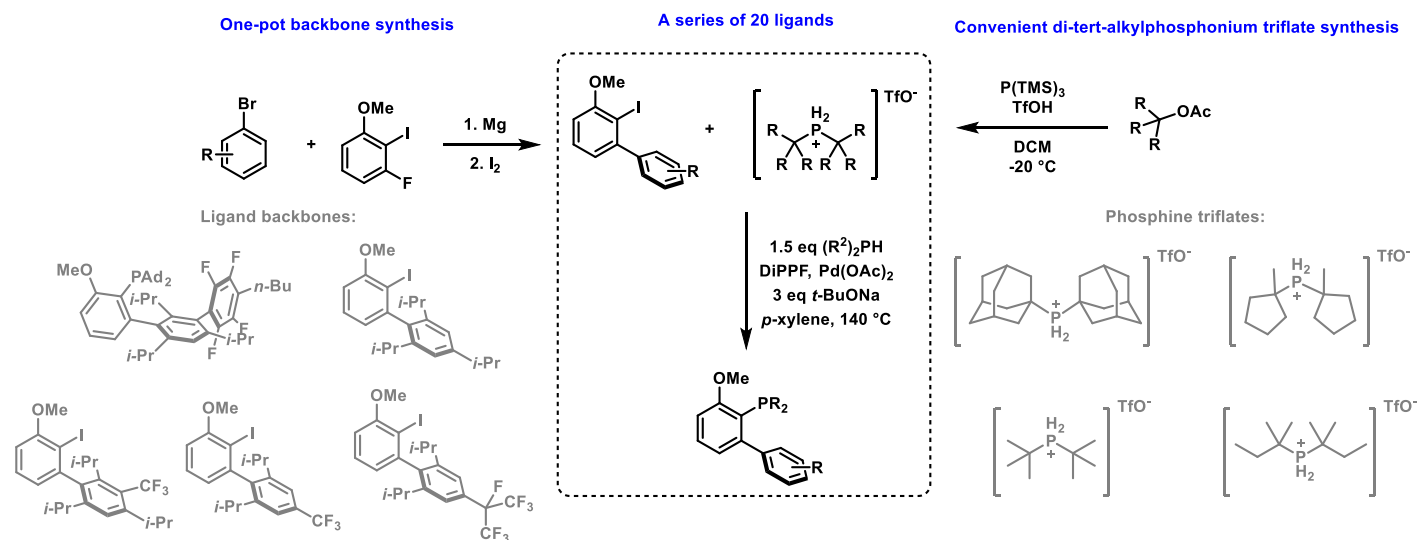
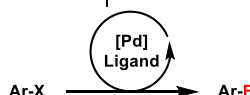
1. Center for Physical Sciences and Technology, Department of Organic Chemistry
Akademijos Str. 7, LT-08412 Vilnius, email: tomas.paskevicius@ftmc.lt

Significant part of research in palladium catalysis has been dedicated to the development of new and more effective phosphine ligands. Among the commonly used and structurally simpler phosphines (trialkyl- and triarylphosphines), biphenyl bearing analogues emerges as a new frontier in the ligand design. Biphenyl backbone can be modified to attain certain desired electronic and steric properties required for more complex types of cross-coupling reactions. More notable studies by Hartwig et. al. suggest that reduced electron density on the palladium atom and increased steric environment around it can aid with more facile reductive elimination step from Pd(II) species [1].

Therefore, in this study we aim to investigate how the introduction of electron withdrawing substituents and t-alkyl motives on phosphorus affect the energetic barrier of the elusive C-F bond formation and thus help in developing more elegant methodologies for the fluorination of electron rich hetero(arenes). This study led to a convenient synthesis of a series of 20 phosphine ligands with differing electronic and steric properties and their initial evaluation in the Pd(II) catalyzed fluorination reaction.

References

- Roy, A. H.; Hartwig, J. F. J. Am. Chem. Soc. 2001, 123, 1232-1233.



Photodarkening in BGSe and BGGSe

Julius Lukošius^{1,2}, Justinas Čeponkus³, Rokas Danilevičius¹, Andrejus Michailovas^{1,2}

1. UAB Ekspla, Savanorių ave. 237, LT-02300 Vilnius, Lithuania
2. Center for Physical Sciences and Technology, Department of Laser technologies
Saulėtekio av. 3, LT-10257 Vilnius, email: julius.lukosiunas@ftmc.lt
3. Institute of Chemical Physics, Vilnius University, Saulėtekio ave. 9, Vilnius, LT-10222, Lithuania

In recent years, the field of middle infrared nonlinear optics has witnessed a growing interest in alternative nonlinear materials alternative to silver gallium sulfide (AGS) crystals, which, despite their widespread use, are hindered by limitations such as a relatively narrow transparency range and susceptibility suffering of to the photodarkening. The emergence of barium gallium selenide (BGSe) and barium gallium germanium selenide (BGGSe) crystals has provided opened a new promising option for in the field of nonlinear optical applications, particularly in the mid-infrared (mid-IR) spectral region [1]. These crystals offer broader transparency ranges extending to longer wavelengths, significantly higher nonlinear coefficients, and superior damage thresholds, making them well-suited for high-power and high-efficiency frequency conversion processes.

The mid-IR region, often referred to as the molecular fingerprint region, holds significant importance for spectroscopy, sensing, and defense applications [2]. Efficient nonlinear conversion across this range is essential for generating broadband pulses and advancing laser technologies. While BGSe and BGGSe crystals exhibit many advantages over AGS, our recent observations reveal that photodarkening, a phenomenon previously associated primarily with AGS, also occurs in these newer materials when exposed to high-energy femtosecond pulses at of a 1030 nm wavelength. Understanding the underlying mechanisms and impacts of this effect is critical important for optimizing the performance and longevity of the BGSe and BGGSe crystals in practical applications.

In this study, we continue our previous work [3] and demonstrate efficient nonlinear conversion using BGSe and BGGSe crystals, achieving broad coverage from 2.3 μm to 10 μm and generating broadband pulses with energies ranging from 1 μJ to 16 μJ at a repetition rate of 1 kHz. Concurrently, we investigate the photodarkening effect observed in these crystals under high-energy femtosecond pumping in the real operational conditions.

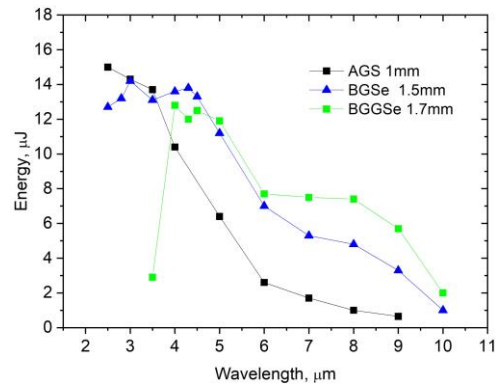


Figure 1. Mid-IR pulse energy throughout the tuning range.

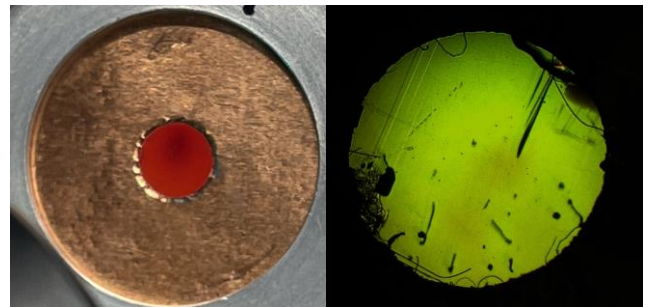


Figure 2. On the left: picture of BGGSe crystal and a dark spot appeared during pumping and mid-IR generation; on the right: microscope picture of BGSe with two permanent dark spots in the middle and lower part of crystal.

References

1. Kostyukova, N., Erushin, E., Boyko, A., Shevyrdyaeva, G., and Badikov, D. (2024). Barium Chalcogenide Crystals: A Review. *Photonics*, 11(3), 281. <https://doi.org/10.3390/photonics11030281>
2. Majid Ebrahim-Zadeh, Amr S. Helmy, Giuseppe Leo, and Peter G. Schunemann, "Mid-infrared coherent sources and applications: introduction," *J. Opt. Soc. Am. B* 40, MIC1-MIC1 (2023)
3. J. Lukošius, R. Kananavičius, R. Danilevičius, R. Januškevičius, P. G. Schunemann, and A. Michailovas, "Efficient high resolution broadband SFG spectrometer utilizing BGSe nonlinear crystal covering 2.5-10 μm spectral range," in *Laser Congress 2023 (ASSL, LAC)*, Technical Digest Series (Optica Publishing Group, 2023), paper ATH2A.4.

SUBMICRON PERIODIC STRUCTURES IN METAL OXIDE THIN FILM VIA LASER ABLATION AND THERMAL OXIDATION

Julianija Nikitina¹, Simonas Indrišiūnas¹, Tomas Tolenis², Mindaugas Andruliavičius³, Lukas Ramalis¹, Lina Grinevičiūtė¹

1. Center for Physical Sciences and Technology, Department of Laser Technologies
Saulėtekio av. 3, LT-10257 Vilnius
2. ELI Beamlines Facility, Extreme Light Infrastructure ERIC, Dolní Břežany, Czech Republic
3. Institute of Materials Science, Kaunas University of Technology, Kaunas, Lithuania email: julianija.nikitina@ftmc.lt

Periodic structures, featuring periodic modulation of optical constants, exhibit polarization control, spectral and angular selectivity of light and thus were found extremely useful for laser radiation manipulation. However, fabrication technologies of periodic surface structures have to face strict requirements: despite a sub-micrometer scale of periodicity required for VIS and IR spectral region applications, the following significant criteria are optical transparency and durability, which require a completely inorganic composition of all constituent materials. Polymers are quite easily processed and can be transparent in the target spectral regions, but they exhibit lower optical resistance than dielectric metal oxides [1]. However, direct patterning of the dielectric materials is challenging at sub-micrometric scale, especially if low surface roughness is required. To get around a direct patterning of metal oxides, a thin metallic layer deposited on a glass substrate can be structured. Subsequent annealing promotes a metal oxidation, producing a fully inorganic, transparent surface structure on a glass substrate.

The fabrication method proposed in this work [2] involves the structuring and subsequent thermal oxidation of a thin metallic layer on a glass substrate, as schematically shown in Fig. 1. Thin tantalum metal films were formed on fused silica substrates using ion beam sputtering technology. Primary step of the investigation was aimed to evaluate optimal oxidation conditions for the structured thin film. For this purpose, the as-deposited metallic samples were thermally annealed in an ambient atmosphere under various conditions. Investigating the structural, optical, and chemical characteristics of various annealed tantalum thin films offered insights into the optimal parameters. Thus, to avoid high optical losses and reach the purest Ta₂O₅ composition, 600 °C annealing temperature and 2 °C/min heating rate were used.

Linear periodic structures – gratings – in thin metallic films were formed via the Direct Laser Interference Writing (DLIP) technique. The two-beam interference pattern was produced from the second harmonic (515 nm wavelength) laser beam of 7-ps short pulses. The resulting period of the linear interference pattern on the sample was 750 nm. After forming the grating structure by DLIP, the last step was annealing to complete metal oxidation, thus forming non-absorbing gratings. The structured films were annealed using the optimal parameters obtained from the investigation of as-grown films. The characterisation of the formed grating structure in thin films, both before and after annealing, involved capturing surface morphology images using an atomic force microscope, which showed increased modulation depths and fill factors. As it is inevitable during the oxidation process, the attachment of oxygen atoms to the metal causes volumetric expansion of the material. Generally, the average modulation depth has increased from 280 to 420 nm, and the fill factor has increased by approximately 10 % for metal oxide structures.

The presented method of direct laser interference patterning of metal layers followed by thermal oxidation by annealing has been proven effective for obtaining sub-micrometer non-absorbing gratings. No absorption has been detected by spectrophotometric measurements, which allows the use of the developed nanostructures for high-intensity laser optics applications. This investigation shows that this method can overcome the problems associated with traditional glass microstructuring and is a promising route for developing advanced optical elements.

References

1. A. Žukauskas, et al., Optical Materials, vol. 39, 2015.
2. J. Nikitina, et al., Applied Surface Science Advances, vol. 24, 2024.

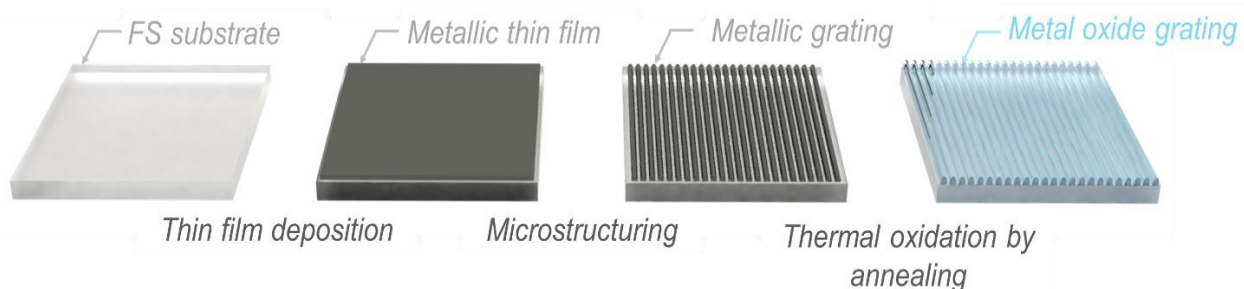


Fig. 1 Manufacturing steps to form metal-oxide submicron gratings from metallic thin film.

Nanostruktūrizuotų dangų stabilizavimas naudojant atominių sluoksnių nusodinimo technologiją

Darija Astrauskytė¹, Lina Grinevičiūtė¹

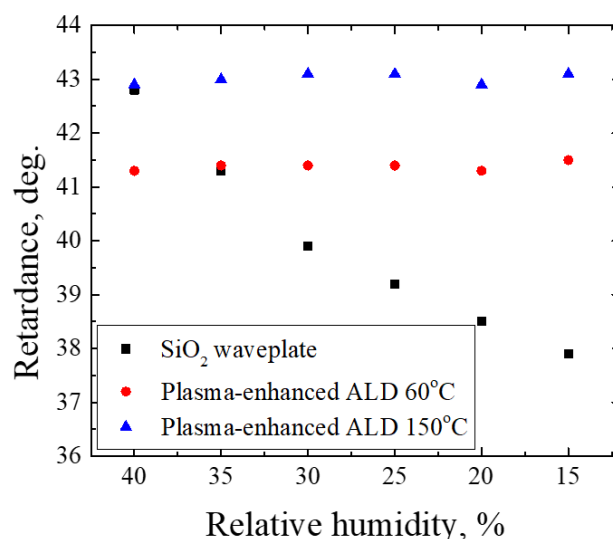
1. Fizinių ir technologijos mokslų centras, Lazerinių technologijų skyrius
Savanorių pr. 231, LT-02300 Vilnius, el. p.: darija.astrauskyte@ftmc.lt

Garinimo kampu (GLAD – angl. k. glancing angle deposition) metodas leidžia valdyti nusodinamų sluoksnių vidinę mikrostruktūrą, porėtumą ir dvejetainiškumą. Dėl šios priežasties kombinuojant tankius ir porėtus sluoksnius galima suformuoti daugiasluoksnes optines dangas tik iš vienos medžiagos. Be to, naudojant medžiagas, kurios pasižymi dideliu atsparumu lazerinei spinduliutei, pavyzdžiui, SiO_2 , galima nusodinti veidrodžius, poliarizatorius ir fazines plokšteles, skirtus didelės galios lazerinėms sistemoms [1–3]. Tačiau dėl porėtumo nanostruktūrizuotos dangos yra jautrios aplinkos pokyčiams – tai yra, kintant aplinkos drėgmei kinta šių dangų efektyvusis lūžio rodiklis, įtempiai ir lazeriu indukuotos pažaidos slenkstis (LIDT – angl. k. laser-induced damage threshold). Taip pat, anizotropinių dangų atveju yra stebimi skirtuminio fazės vėlinimo pokyčiai priklausantys nuo aplinkos drėgmės.

Vandens garų adsorbciją į porėtą struktūrą gali sustabdyti tankus apsauginis sluoksnis, kuris izoliuotų porėtą dangą nuo aplinkos ir stabilizuotų jos optines charakteristikas. Atominių sluoksnių nusodinimas (ALD – angl. k. atomic layer deposition) yra perspektyvi technologija apsauginių sluoksnių formavimui ant nanostruktūruotų anizotropinių dangų. ALD metodas leidžia suformuoti tankius ir tolygius sluoksnius ant sudėtingos formos pagrindų [4]. Be to, ploni ALD sluoksniai yra taikomi apsauginių dangų formavimui ant polimerų ir porėtų sluoksnių [5].

Šiame darbe anizotropinės SiO_2 dangos buvo nusodintos naudojant elektronų pluošto garinimo kampu metodą. 150 nm storio apsauginiai Al_2O_3 sluoksniai buvo suformuoti naudojant ALD technologiją oksidatoriumi naudojant deguonies plazmą 60°C ir 150°C temperatūrose. Anizotropinių dangų skirtuminis fazės vėlinimas buvo nustatytas naudojant dvejetainiškumo vaizdinimo sistemą 488 nm bangos ilgyje. Anizotropinių dangų stabilumas prieš ir po apsauginių sluoksnių nusodinimo buvo įvertintas stebint skirtuminio fazės vėlinimo kitimą keičiant aplinkos santykinę drėgmę.

Prieš apsauginių sluoksnių nusodinimą anizotropinių SiO_2 dangų skirtuminis fazės vėlinimas sumažėjo nuo 43° iki 38°, kai santykinė aplinkos drėgmė sumažėjo nuo 40% iki 15% (1 paveikslas). Po apsauginių Al_2O_3 sluoksnių nusodinimo anizotropinių dangų skirtuminis fazės vėlinimas išliko nepakitęs, nepriklausomai nuo aplinkos drėgmės.



1 paveikslas. Anizotropinių dangų skirtuminio fazės vėlinimo priklausomybė nuo santykinės aplinkos drėgmės prieš ir po apsauginių sluoksnių nusodinimą.

Literatūra

1. Grinevičiūtė, L.; Andrulevičius, M.; Melninkaitis, A.; Buzelis, R.; Selskis, A.; Lazauskas, A.; Tolenis, T. Highly Resistant Zero-Order Waveplates Based on All-Silica Multilayer Coatings. *Physica Status Solidi (a)* **2017**, *214*, 1700764.
2. Grinevičiūtė, L.; Ramalis, L.; Buzelis, R.; Tolenis, T. Highly Resistant All-Silica Polarizing Coatings for Normal Incidence Applications. *Opt. Lett.* **2021**, *46*, 916.
3. Tolenis, T.; Grinevičiūtė, L.; Smalakys, L.; Ščiuka, M.; Drazdys, R.; Mažulė, L.; Buzelis, R.; Melninkaitis, A. Next Generation Highly Resistant Mirrors Featuring All-Silica Layers. *Sci Rep* **2017**, *7*, 10898.
4. Astrauskytė, D.; Galvanauskas, K.; Gailevičius, D.; Drazdys, M.; Malinauskas, M.; Grinevičiūtė, L. Anti-Reflective Coatings Produced via Atomic Layer Deposition for Hybrid Polymer 3D Micro-Optics. *Nanomaterials* **2023**, *13*, 2281.
5. Ma, P.; Pu, Y.; Zhang, W.; Die, J.; Zhang, M.; Liu, H. Protecting the EBE Coatings from Vacuum-Air-Shift by Ion Assistance or ALD Capping Layer. *Ceramics International* **2022**, *48*, 2670–2676.

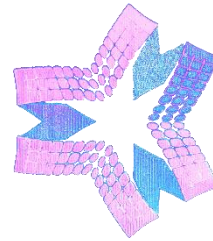
LAZERINIS NANODALELIŲ GENERAVIMAS IŠ Ti-Au PLONŲ DANGŲ PLAZMONINIŲ SPALVŲ ANALIZEI

Vita Petrikaitė¹, Aušra Selskienė¹, Evaldas Stankevičius¹

1. Fizinių ir technologijos mokslų centras, lazerinių technologijų skyrius
Savanorių per. 231, LT-02300 Vilnius, el. p.: vita.petrikaite@ftmc.lt

Įprasti sintetiniai dažai pasižymi plačiu spalvų spektru, tačiau dažnai kelia ekologinę grėsmę dėl toksiškų ir biologiškai neskaidomų medžiagų išsiskyrimo [1]. Plazmoninės nanostruktūros, ypač auksinės nanodalelės, siūlo tvarią alternatyvą dėl unikalių optinių savybių. Keičiant metalo nanodalelių dydį, formą ir sudėtį, galima reguliuoti jų šviesos sugerties ir sklaidos savybes, kad būtų sukurtos specifinės spalvos. Skirtingai nuo įprastinių struktūrinių spalvų, kurios priklauso nuo nanostruktūrų periodiškumo, lemiančio matomą spalvą [2], plazmoninės spalvos sukuriamos dėl lokalizuotų rezonansų atskirose nanostruktūrose. Plazmonika grindžiama koherentiniais laidumo juostos elektronų virpesiais nanodalelėse, vadinamaisiais plazmonais [3]. Lokalizuotieji paviršiaus plazmonų rezonansai (LPPR) apibūdina šviesos ir metalo nanodalelių sąveiką, apimančią krūvio tankio svyravimus nanodalelių paviršiuje [4]. Ryškios plazmoninių nanodalelių spalvos skiriasi nuo tūrinių medžiagų atspalvių. Tačiau termiškai generuojamos nanodalelės lazeriu iš plonos aukso dangos pasižymi ribotu spalvų diapazonu dėl morfologinių apribojimų [5]. Šiame darbe siekta išplėsti plazmoninių spalvų spektrą įterpiančią adhezinį titano (Ti) pasluoksnį tarp stiklo padėklo ir aukso dangos. Šis sluoksnis skirtas pagerinti tiek aukso plazmoninių spalvų įvairovę, tiek dangos stabilumo savybes [6].

Eksperimentai atlikti nanodaleles generuojant iš plonų dangų (Au 8 nm; Ti 2 nm + Au 8 nm; Ti 4 nm + Au 8 nm; Ti 6 nm + Au 8 nm; Ti 10 nm + Au 10 nm; Au 8 nm + Ti 6 nm) jas termiškai kaitinant nanosekundiniu impulsiniu lazeriu, veikiančiu 532 nm bangos ilgio diapazone. Sisteminė analizė buvo atlikta keičiant impulso energiją (3,5 μ J – 38,5 μ J), skenavimo greitį (1 mm/s – 500 mm/s), pasikartojimo dažnį (0,5 kHz–10 kHz) ir linijų tarpą (25 μ m – 75 μ m), siekiant optimizuoti lazerio parametrus plazmoninių spalvų formavimui. Nustatyta, kad dangos su Ti pasluoksniu pasižymėjo intensyvesnėmis lokalizuoto paviršiaus plazmonų rezonanso (LPPR) smailėmis. Sluoksnių konfigūracija Ti 10 nm + Au 10 nm pasižymėjo plačiausiu spalvų spektru, su maksimaliu spalvų skirtumo parametru $\Delta E = 36,83$, ir aukštomis ekstinkcijos vertėmis, net esant mažai impulsų energijai. Nustatyta, kad didinant Ti pasluoksnio storį, vyksta raudonasis poslinkis ilgesnių bangų link ir mažėja reikalinga impulso energija spalvai gauti. Šie rezultatai patvirtina, kad nanodalelės generuotos iš plonų Ti/Au dangų naudojant lazerinį terminį kaitinimą yra perspektyvus metodas plazmoninėms spalvinėms savybėms gauti be litografijos, kurios pritaikomos didelės raiškos spausdinimui, apsaugai nuo klastojimo, fotoninių komponentų ir ekologiškų optinio spausdinimo technologijų taikyme.



CENTER
FOR PHYSICAL SCIENCES
AND TECHNOLOGY

1 pav. Optinės mikroskopijos nuotrauka, kurioje matomas šio tyrimo metu sugeneruotas Fizinių ir technologijos mokslų centro logotipas.

Literatūra / References

1. J. Lin, W. Ye, M. Xie, D.H. Seo, J. Luo, Y. Wan, B. Van der Bruggen, Environmental impacts and remediation of dye-containing wastewater, *Nature Reviews Earth & Environment* 4 (2023) 785-803.
2. Q. Chen, D.R. Cumming, Visible light focusing demonstrated by plasmonic lenses based on nano-slits in an aluminum film, *Optics Express* 18 (2010) 14788-14793.
3. D. Bohm, D. Pines, A collective description of electron interactions. I. Magnetic interactions, *Physical Review* 82 (1951) 625.
4. C.F. Bohren, D.R. Huffman, *Absorption and scattering of light by small particles*, John Wiley & Sons 2008.
5. V. Petrikaitė, G. Niaura, E. Stankevičius, et al. Hybrid gold-silver nanoparticles synthesis on a glass substrate using a nanosecond laser-induced dewetting of thin bimetallic films and their application in SERS. *Opt Laser Technol.*, 168, 109956 (2024).
6. R. Liudvinavičius, A. Selskis, E. Stankevičius. Titanium adhesion layer influence on the formation of hybrid lattice plasmon structures via laser-direct writing. *Optics & Laser Technology*, 175, 110807 (2024).

HIBRIDINĖS SIDABRO-AUKSO BIMETALINĖS NANOGRADDELĖS, SKIRTOS PLAZMONŲ REZONANSO SENSORIKAI

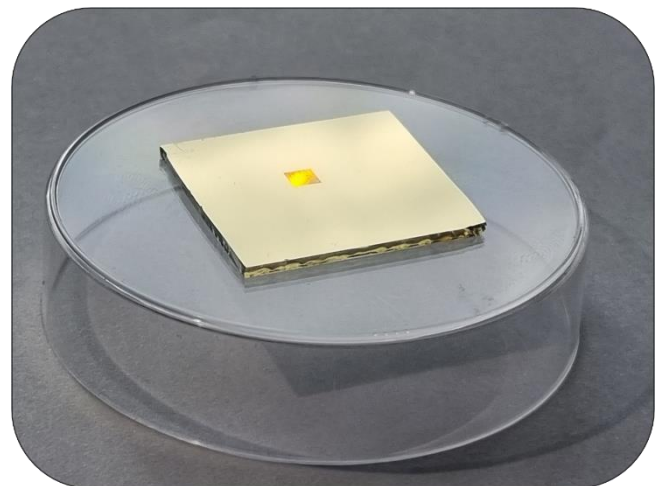
Kernius Vilkevičius¹, Tomas Rakickas², Evaldas Stankevičius¹

1. Fizinių ir technologijos mokslų centras, Lazerinių technologijų skyrius
Savanorių pr. 231, LT-02300 Vilnius, el. p.: kernius.vilkevicius@ftmc.lt
2. Fizinių ir technologijos mokslų centras, Nanoinžinerijos skyrius
Savanorių pr. 231, LT-02300 Vilnius

Tiesioginis lazerinis rašymas suteikia galimybę greitai ir tiksliai femtosekundiniais impulsais suformuoti periodinius nanodarinius plonose sidabro ar aukso dangose. Tikslus pozicionavimas bei impulso energijos valdymas leidžia suformuoti didele tvarka ir vienodumu pasižyminčią dvimatę metalinę gardelę. Aukso dangoje suformuotos struktūros pasižymi plačia morfologine įvairove, kai tuo tarpu sidabrinės struktūros pasižymi stipresnėmis plazmoninėmis savybėmis. Sidabro-aukso bimetalinės dangos panaudojimas leidžia išnaudoti abiejų metalų privalumus – suformuoti stipriomis plazmoninėmis savybėmis pasižyminčias skirtingų formų struktūras. Nanoantenos su aštriomis viršūnėmis itin sustiprina lokalų elektrinį lauką, tad ši morfologija tinkama pritaikyti paviršiumi sustiprintoje Ramano spektroskopijoje [1,2]. Tuo tarpu pussferės formos nanogumbeliai sužadina ir apjungia plazmonines modas, kurių rezonansas tinkamas pritaikyti sensorikoje. Pastaruoju atveju spektre matoma siaura rezonansinė smailė, kurios spektrinė pozicija priklauso nuo aplinkos lūžio rodiklio. Didėjant lūžio rodikliui, smailė slenka į raudonąją spektro sritį, o poslinkio vertė leidžia nustatyti lūžio rodiklio pokytį arba tiriamo skysčio ar dujų koncentraciją [3].

Tyrimo metu buvo formuojamos periodinės nanogumbelių gardelės 50 nm sidabro, aukso bei sidabro-aukso bisluoksnio dangose (1 pav.) ir tiriamas jų sužadinto plazmono rezonanso atsakas lūžio rodiklio pokyčiui. Struktūros formuotos naudojant 343 nm bangos ilgio femtosekundinį lazerį, o plazmoninis atsakas matuotas spektrofotometru. Jutiklio jautrumo nustatymui naudoti 5 skysčiai – dejonizuotas vanduo (lūžio rodiklis $n = 1.3314$) bei 1.7% ($n = 1.3339$), 3.4% ($n = 1.3364$), 5.1% ($n = 1.3389$) ir 6.8% ($n = 1.3414$) koncentracijų glicerolio tirpalai. Ant suformuotos gardelės matavimams pritvirtinta adhesinė kamera, į kurios vidų buvo įleidžiamas matuojamas skystis. Palyginus gryno aukso, gryno sidabro bei sidabro-aukso bisluoksnio gardeles buvo nustatyta, kad nors didžiausiu stiprinimu pasižymi sidabriniai dariniai, geriausią kokybės ir ilgaamžiškumo santykį turi bei praktiniams pritaikymams labiau tinkami bimetaliniai dariniai dėl jų atsparumo oksidacijai. Matuojant rezonanso atsaką skirtingos koncentracijos skysčiams, pastebėtas smailės poslinkis į didesnius bangos ilgius kas 2-3 nm, lūžio rodikliui kintant kas 0.0025, kas nusako tokios platformos jautrumą artimą 800 nm/RIU. Palyginus skirtingos kilmės rezonansines smailes, pastebėta, jog kiekviena jų pasižymi skirtingu jautrumu, kuris priklauso nuo naudojamos krentančios spinduliuotės poliarizacijos. Papildomai tiriant bisluoksninio darinio sensorines galimybes ties skirtingais spinduliuotės kritimo kampais, buvo nustatyta, jog tokiu būdu galima

dar padidinti smailės poslinkį ir jautrumą, pasiekiant 933 nm/RIU vertes. Tuo tarpu kokybės parametras FOM (angl. *Figure of Merit*) tam tikriems rezonansams taip pat pagerinamas atliekant matavimus ties didesniais kampais ir pasiekama 57 RIU⁻¹ vertė. Galiausiai nustatytas tokios jutiklio platformos atkartojamumas bei ilgaamžiškumas. Atlikus matavimus po pusės metų, išmatuoti rezultatai buvo itin artimi gautiems tik suformavus gardelę. Tai parodo, jog šis laisvos formos bei greitai suformuojamas jutiklis yra tinkamas ne tik tikslams, bet ir ilgalaikiams matavimams.



1 pav. Bimetalinis plazmoninis jutiklis.

Literatūra

1. Z.-Y. Li, Adv. Opt. Mater. 6, 1701097 (2018).
2. K. Vilkevičius, I. Ignatjev, A. Selskis, G. Niaura, E. Stankevičius, Appl. Surf. Sci. 660, 160003 (2024).
3. F. Inci, Y. Saylan, A. M. Kojouri, M. G. Ogut, A. Denizli, and U. Demirci, Appl. Mater. Today 18, 100478 (2020).

AUKSO IR SIDABRO MIKROGUMBELIŲ GARDELĖS ŽADINANČIOS PLAZMONŲ REZONANSĄ

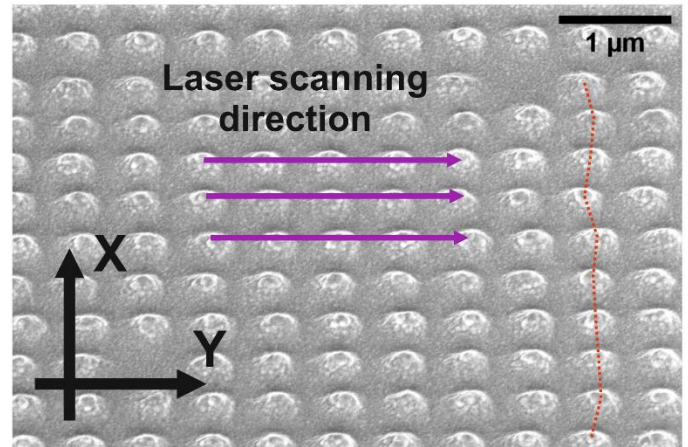
Rodrigas Liudvinavičius¹, Evaldas Stankevičius¹

1. Fizinių ir technologijos mokslų centras, Lazerinių technologijų skyrius
Savanorių per. , LT-02300 Vilnius, el. p.: rodrigas.liudvinavicius@ftmc.lt

Pastaruoju metu plazmonikos kryptis vis labiau sulaukia dėmesio dėl sėkmingo nanostruktūrų taikymo įvairiose srityse – nuo biologinių jutiklių kūrimo ir plazmoninio lazeriavimo (įskaitant aukštesniųjų harmonikų generavimą) iki paviršiumi sustiprintos Ramano sklaidos, taip pat ženklinimo nuo klastojimo ar naujų optinių įrenginių vystymo [1]. Tokį susidomėjimą lemia ypatinga savybė – paviršinių plazmonų rezonansas, atsirandantis kaip kolektyviniai elektronų svyravimai, sužadinti krintančios elektromagnetinės bangos. Šis reiškinys leidžia pasiekti itin stiprią elektromagnetinio lauko lokalizaciją nanomasteliu, kuri yra būtina daugelio plazmoninių rezonansu grįstų sistemų veikimui.

Įprastai šis efektas pasiekiamas naudojant difrakcinius reiškinius. Vienas jų realizuojamas pasitelkiant Kretschmann konfigūraciją, kai naudojama prizmė, suderinanti krintančią šviesą su paviršinio plazmono banga. Tiesioginis lazerinis rašymas leidžia šį efektą gauti tiesiai ant paviršiaus, be papildomų optinių komponentų, kuomet difrakcinis reiškinys išpildomas periodiškai išdėstant mikrostruktūras. Reikšmingą postūmį plazmonikos plėtrai suteikė ir lazerinės technologijos, ypač jau minėtas tiesioginis lazerinis rašymas (TLR), tapęs patrauklia alternatyva tradiciniams litografijos būdams. TLR metodas leidžia formuoti mažesnius nei 1 μm darinius tiesiogiai ant metalinių paviršių, nereikalaudant didelių gamybos išlaidų ir ilgo pasirengimo proceso, kaip litografijos atveju. Naudojant TLR, periodiškai formuojamos metalo mikrostruktūros gali tiesiogiai paviršiuje sužadinti plazmonų rezonansą. Šis metodas yra lankstesnis, nes suteikia galimybę keisti struktūrų parametrus gamybos metu, ir efektyvesnis, nes leidžia žadinti hibridinės gardelės plazmonų modą, t. y. vienu metu sužadinti kelias skirtingas modas. Tai lemia siauresnius ir gilesnius rezonansus, kurie atveria dar daugiau naujų galimybių praktiniams taikymams.

Šiame darbe bus aptartos aukso ir sidabro periodinės mikrogumbelių gardelės, žadinančios hibridinės gardelės plazmonų rezonansą. Bus nagrinėjamos tiesioginio lazerinio rašymo metodo galimybės kuriant mikrostruktūras, aptariamos jų formos ir dydžiai, technologinės galimybės bei formavimo apribojimai. Taip pat bus analizuojami skirtingų taurių metalų panaudojimai ir jų praktiniai aspektai, o galiausiai – tiesiogiai palyginti vienodo periodo aukso ir sidabro mikrogumbelių gardelių rezultatai, atskleidžiant plazmonų žadinimo ypatumus, jų priklausomybę nuo struktūros parametrų bei pasiekiamas rezonansų charakteristikas.



1 pav. Sidabro mikrogumbelių struktūrų suformuotų plonoje sidabro dangoje SEM nuotrauka.

Literatūra

1. K. Yang, X. Yao, B. Liu, B. Ren, Metallic Plasmonic Array Structures: Principles, Fabrications, Properties, and Applications. Adv. Mater. 33(50), pp. 2007988 (2021).
2. R. Liudvinavičius, A. Selskis, E. Stankevičius, Titanium adhesion layer influence on the formation of hybrid lattice plasmon structures via laser-direct writing, Optics & Laser Technology, Volume 175, 2024.
3. R. Liudvinavičius, K. Vilkevičius, E. Stankevičius, High-quality grating-coupled surface plasmon resonances in silver and gold bumps arrays fabricated in thin metallic films using the third harmonic of femtosecond laser, Applied Surface Science, Volume 711, 2025.

Mechanical and Thermal Property Optimization of SiC-Reinforced AlSi10Mg Composites via DMLS

Karolis Stravinskas¹, Ada Steponavičiūtė¹, Ričardas Petkus¹, Genrik Mordas¹

1. Center for Physical Sciences and Technology, Department of Laser Technologies
Saulėtekio av. 3, LT-10257 Vilnius, email: vardas.pavarde@ftmc.lt

Additive manufacturing has changed the production for complex geometries and custom parts, allowing layer by layer fabrication of parts with design freedom. While polymer based additive manufacturing has matured fast, ceramic and metal based systems have unique challenges due to high melting points, brittleness and sensitivity to processing parameters. Ceramic materials are valued for their hardness, thermal stability and chemical resistance but have been difficult to process using conventional additive manufacturing techniques. However, integrating ceramic reinforcements into metal matrices through processes like Direct Metal Laser Sintering (DMLS) offers a way to create advanced composite materials that combine the ductility of metals with the superior mechanical and thermal properties of ceramics. This study investigates the effect of 10% Silicon Carbide (SiC) reinforcement on the mechanical and thermal properties of AlSi10Mg manufactured by DMLS. The research optimized laser energy density to study the effect on density, hardness, surface roughness, tensile strength and thermal behaviour. A comparison between unreinforced AlSi10Mg and SiC reinforced AlSi10Mg shows the complex interactions between laser processing parameters, thermal conductivity and phase stability. The introduction of SiC changes the material's response to laser energy, affecting melt pool dynamics, solidification behaviour and residual stress formation.

The results show SiC reinforcement improves hardness and wear resistance but increases thermal stresses, so precise process control is needed to avoid defects like porosity, microcracking and SiC decomposition. The composite also has a shift in optimal process parameters due to changed thermal conductivity, laser absorption and powder bed packing density compared to the base alloy. These findings highlight the need to balance laser power, scan speed and hatch spacing to get a defect free structure with the desired mechanical and thermal properties. This study provides insights into the role of SiC in Metal Matrix Composites (MMCs) and practical guidelines to refine DMLS parameters to obtain the optimal combination of strength, hardness, ductility, and thermal stability in SiC-reinforced AlSi10Mg parts. The results contribute to the understanding of MMCs for high-performance applications in aerospace, automotive, and thermal management systems.

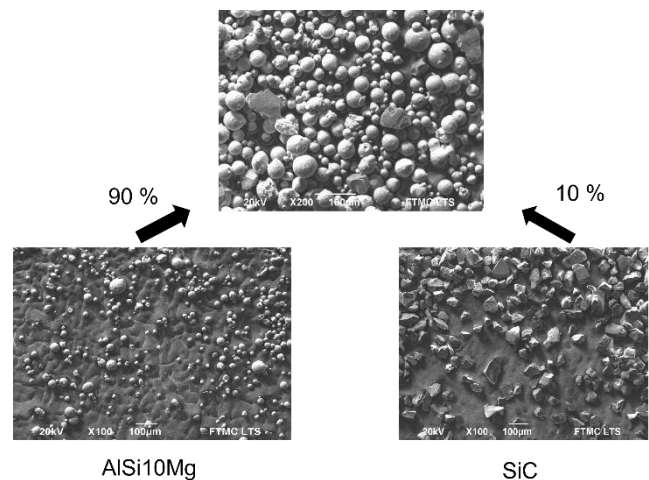


Fig. 1. SEM images of powders used for DMLS: AlSi10Mg and SiC

Design and Investigation of SSAIL Transparent Electrodes on Glass for Electrochromic Applications

Dainius Balkauskas¹, Titas Tamošauskas¹, Modestas Sadauskas¹, Romualdas Trusovas¹, Karolis Ratautas¹, Alexandr Belosludtsev¹

1. Centre for Physical Sciences and Technology, Department of Laser Technologies

Saulėtekio av. 231, LT-02300 Vilnius, email: dainius.balkauskas@ftmc.lt

We present a cost-effective and scalable method for fabricating transparent microscale metal electrodes on glass substrates using laser-induced metal deposition (SSAIL) technology. These innovative electrodes function as efficient conductive layers for electrically tunable electrochromic devices, such as smart windows, variable filters, and sensors. This study explores the process of electrode formation and evaluates various design configurations. Furthermore, we compare the performance of microscale copper lines fabricated with SSAIL to that of traditional transparent and electrically conductive indium tin oxide (ITO) electrodes. The results demonstrate that SSAIL-fabricated electrodes achieve an optimal balance between electrical conductivity and optical transparency, outperforming ITO electrodes.

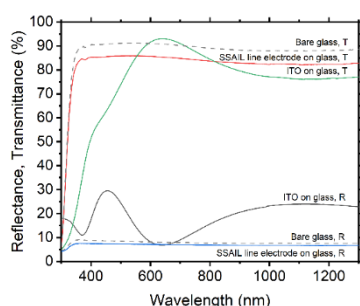


Fig. 1. Transmittance (T) and Reflectance (R) spectra of transparent and electrically conductive ITO and SSAIL line micro-scale copper electrodes.

Furthermore, the optimized copper electrode design was tested in a multilayer electrochromic device structure.

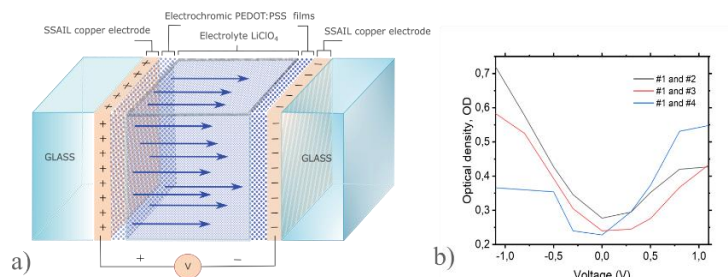


Fig. 2. a) battery type SSAIL-based electrochromic device scheme, b) Optical density dependence from voltage of different thickness PEDOT:PSS coating.

It used a flexible conductive polymer, Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), in combination with the Lithium perchlorate (LiClO_4) electrolyte [3]. We showed how the proper layer alignment is important for the final device performance. The electrochromic effect investigation confirms that such copper electrodes

work well as electrodes for an electrochromic device. The optical density changed from 0.27 to 0.72. Our findings suggest that transparent microscale electrodes formed by laser-induced metal deposition could contribute to developing more sustainable and cost-effective smart devices.

References

1. M. Sadauskas, V. Vrubliauskaitė, E. Kvietkauskas, D. Balkauskas, R. Trusovas, A. Belosludtsev, K. Ratautas, Microscale copper traces by laser induced copper deposition on glass and PET substrate, *Opt. Laser Technol.* 161 (2024) 112355. <https://doi.org/10.1016/j.optlastec.2024.112355>.
2. Dainius Balkauskas, Evaldas Kvietkauskas, Modestas Sadauskas, Viktorija Vrubliauskaitė, Romualdas Trusovas, Karolis Ratautas, Alexandr Belosludtsev, Transparent microscale electrodes formed by laser-induced metal deposition on glass for smart windows application, *Optics & Laser Technology*, <https://doi.org/10.1016/j.optlastec.2025.113669>.
3. J.Y. Kim, J.-Y. Oh, S. Cheon, H. Lee, J. Lee, J.-I. Lee, H. Ryu, S.M. Cho, T.-Y. Kim, C.-S. Ah, Y.-H. Kim, C.-S. Hwang, Optimized ion diffusion depth for maximizing optical contrast of environmentally friendly PEDOT:PSS electrochromic devices, *Opt. Mater. Express* 6 (2016) 3127–3142. <https://doi.org/10.1364/OME.6.003127>.

Two-Photon Polymerization of Low-Density Micro-Targets and Assembly into Rigid Holders for Inertial Confinement Fusion Studies

Ioanna Petsi^{1,3}, Saule Petrauskaite¹, Dimitra Ladika¹, Donatas Narbutis², Mangirdas Malinauskas¹

1. Vilnius University, Laser Research Center, Vilnius, Lithuania

2. Vilnius University, Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania

3. University of Patras, Faculty of Physics, Patra, Greece

One of the major topics of research of the last decades is Two-Photon Lithography (TPL), which is a non-linear laser direct writing technique that is based on two-photon absorption phenomenon.[1] It provides sub-diffraction features and it can be used to create complex, true 3D-printed micro and porous structures[2], without the need of using masks. TPL is often used for the fabrication of different geometries, like foams. High porosity foams have many applications in optics and photonics, biology, mechanics, acoustics, electronics etc.[1]

One of the properties that make them really significant is their ability to produce plasma during Inertial Confinement Fusion (ICF)[3], which is a method of achieving nuclear fusion by using lasers or other energy sources to compress and heat a small fuel pellet until it implodes and fuses. The main requirements of the microstructures in order to be used as targets, are low and uniform density[3], as well as the absence of more heavy elements than Carbon.

The aim of this work is to fabricate low-density woodpile geometry foams of acrylate materials using TPL, employing a 517 nm femtolaser source. Specifically, the materials that were used were (PETA:PETTA)(60:40) and photoinitiator 0.5% thioxanthone-9h, which is a chemical compound that absorbs light and produces reactive species, such as free radicals, to initiate polymerization. The achieved density was 0.07% g/cm³. The woodpiles were also tested mechanically. Finally, the woodpiles were integrated into a 3D printed holder, which is easy handling during ICF experiments, that will be conducted at ABC group of ENEA in Frascati by dr. Mattia Cipriani.

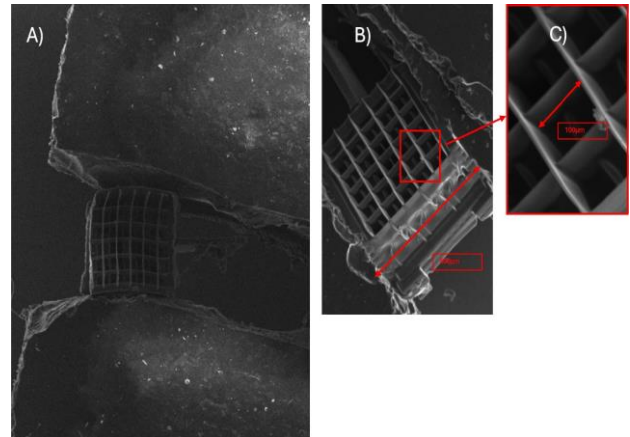


Figure 1: Scanning Electron Microscope (SEM) pictures of A) high-porosity woodpile microstructures integrated into the holder. B) Magnified woodpile inside the 3D printed holder. C) Magnified woodpile inside the 3D printed holder. The estimated density of the structure is 0.07% g/cm³. The distance between the filaments is 100 μ m. The woodpile has dimensions 500 μ m in X and Y axis and 250 μ m in Z axis.

References

1. Wang, H., Zhang, W., Ladika, D., Yu, H., Gailevičius, D., Wang, H., Pan, C.-F., Nair, P. N. S.,
2. Ke, Y., Mori, T., Chan, J. Y. E., Ruan, Q., Farsari, M., Malinauskas, M., Juodkasis, S., Gu, M., Yang, J. K. W., Two-Photon Polymerization Lithography for Optics and Photonics: Fundamentals, Materials, Technologies, and Applications, Advanced Function Materials, 2023.
3. Skliutas, E., Lebedevaite, M., Kabouraki, E., Baldacchini, T., Ostrauskaite, J., Vamvakaki, M., Farsari, M., Juodkasis, S., Malinauskas, M., Polymerization mechanisms initiated by spatio-temporally confined light, De Gruyter Brill, 2021.
4. Cipriani, M., Consoli, F., Scisciò, M., Solovjovas, A., Petsi, I. A., Malinauskas, M., Andreoli, P., Cristofari, G., Experimental and theoretical study on high-power laser irradiation of 3D-printed micro-structures at the ABC laser facility, High Power Laser Science and Engineering, Submitted.

DESIGN OF WIDE INPUT VOLTAGE RANGE DC-DC CONVERTER INTEGRATED CIRCUIT FOR AUTOMOTIVE APPLICATIONS

Lukas Šalavėjus¹, Vaidotas Barzdėnas¹, Aleksandr Vasjanov¹, Tzung-Je Lee²

1. Department of Computer Science and Communications Technologies, Vilnius Gediminas Technical University, Vilnius, email: lukas.salavejus@vilniustech.lt
2. Institute of Integrated Circuit Design, Department of Electrical Engineering, National Sun Yat-Sen University, Kaohsiung, Taiwan

The integration of advanced electronic modules such as GNSS (Global Navigation Satellite System) trackers, Wi-Fi units, and cellular modems has become increasingly prevalent in modern automotive electronics. These devices, which rely on communication standards including 2G, 3G, 4G, and 5G, generally require a stabilized 4 V supply and consume currents in the range of 0.1 A to 2 A [1]. Since vehicle battery voltages can vary widely – from 12 V to as high as 48 V – there is a clear need for DC-DC converters with wide input capability to ensure stable power delivery. This makes such converters adaptable across diverse vehicle categories, from conventional passenger cars to electric scooters and bicycles [2]. The present research addresses gaps in the field by evaluating converter solutions optimized for low-power automotive systems, from GNSS trackers [3] to vehicle-to-everything (V2X) [4] communication modules.

The objective of this work is to design a high-efficiency DC-DC buck converter suited for a wide range of automotive applications, supporting 12 V, 24 V, and 48 V battery systems. Managing this variety of input voltages introduces significant design challenges, especially when aiming to guarantee consistent operation, reliability, and cost-effectiveness across multiple vehicle platforms.

The research begins with an analysis of commercially available converter implementations to determine the most appropriate control strategy. From this assessment, the asynchronous buck topology employing Constant On-Time (COT) control was chosen, as it combines structural simplicity with rapid transient performance and effective handling of wide input voltage ranges [5].

The high-level architecture of the proposed system is illustrated in Fig. 1. It is based on an asynchronous buck converter topology, where an integrated power MOSFET generates high-voltage pulses at the output stage. The output voltage is then regulated by averaging pulses over the duty cycle, enabling the input voltage to be stepped down to the required level.

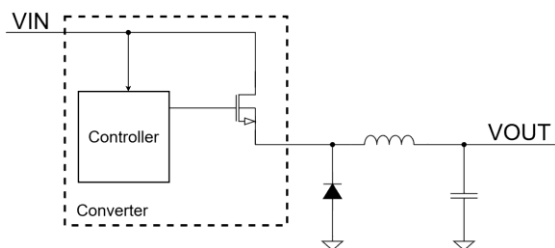


Fig. 1. High-level architecture of the designed DC-DC converter

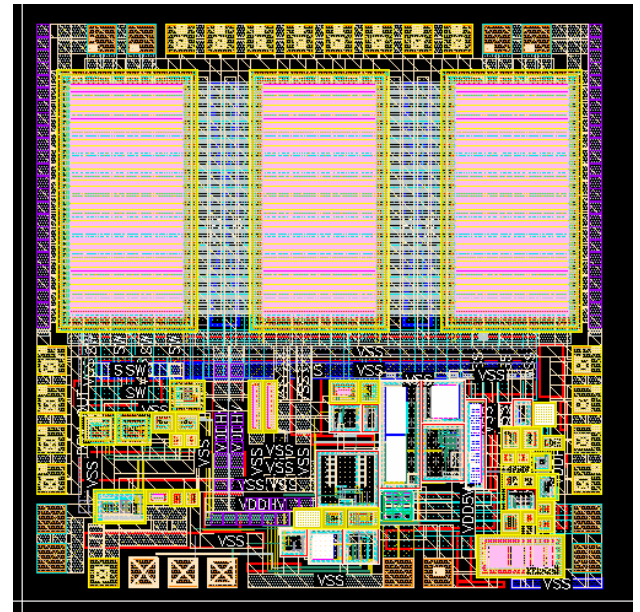


Fig. 2. Design of proposed DC-DC integrated circuit

results indicate that the converter operates reliably across a temperature range of $-40\text{ }^{\circ}\text{C}$ to $+125\text{ }^{\circ}\text{C}$ with an input voltage spanning from 8 V to 60 V, while delivering up to 2 A load current at a regulated 4 V output. The peak efficiency reaches 91.31%, and across the entire input voltage range, the efficiency remains above 87% at full load (2 A, 4 V output).

References

1. C.B.B. De Souza, et al. Analysis of Power Consumption in 4G VoLTE and 5G VoNR Over IMS Network, Proceedings of the 2022 IEEE 27th International Workshop on Computer Aided Modeling and Design of Communication Links and Networks (CAMAD), 2022: 59–64.
2. Texas Instruments. Automotive Power Conversion: 48-V Battery Systems Are the Future of Mild Hybrid Electric Vehicles, White Paper SLYY243, 2018.
3. L. Yin, et al. A GNSS/5G Integrated Positioning Methodology in D2D Communication Networks, IEEE Journal on Selected Areas in Communications, 2018, 36: 351.
4. K. Kiela, et al. Review of V2X-IoT Standards and Frameworks for ITS Applications, Applied Sciences, 2020, 10: 4314.
5. L. Šalavėjus, et al. An Experimental Review of Step-Down Converter Topologies with Wide Input Voltage Range for Modern Vehicle Low-Power Systems, Electronics, 2025, 14: 1712.

The designed integrated circuit occupies an area of $1.5 \times 1.5\text{ mm}^2$ area, as shown in Fig. 2. Simulation

STAR CLUSTER SIZE EVOLUTION IN THE ANDROMEDA GALAXY

Karolis Daugevičius¹, Rima Stonkutė¹, Vladas Vansevičius¹

1. Center for Physical Sciences and Technology, Department of Fundamental Research
Saulėtekio av. 3, LT-10257 Vilnius, email: karolis.daugevicius@ftmc.lt

Star clusters (SCs) are fundamental building blocks of galaxies. The majority of newborn stars form in clustered environments [1], most of which eventually dissolve into the field stellar population of their host galaxies [2]. The structural evolution and dissolution of SCs are driven by a variety of mechanisms, including internal cluster dynamics, stellar evolutionary feedback, and external tidal or dynamical perturbations, such as galactic fields, spiral arms, or giant molecular clouds. Studies of the SCs' structure and size changes with age in different environments provide key constraints on theoretical models, helping us to better understand the physical processes driving cluster evolution, determining survival timescales, and shaping the build-up of the field stellar populations in host galaxies.

The Andromeda galaxy (M31) is an ideal target for studying star clusters at high resolution. Its proximity, combined with the capabilities of modern space-based observatories, enables us to resolve individual stars and directly link cluster-scale properties to galaxy-wide processes. Moreover, as the nearest large spiral galaxy similar to the Milky Way, M31 provides a crucial laboratory for understanding the Galaxy.

Our study is based on data from the Panchromatic *Hubble* Andromeda Treasury (PHAT) survey [3], performed with the *Hubble Space Telescope*. We use the M31 SCs catalogue [4], which includes physical parameters (age, mass, and extinction) as well as structural parameters, derived from integrated aperture photometry measurements.

In Fig. 1, we show evolution of the SC half-light radii R_h with cluster ages. We find that the most rapid R_h change occurs during the first ~40 Myr – the median value increases by more than two times. We demonstrate that our findings for the SC population in the north-eastern part of the M31 disc agree well with theoretical SC evolutionary models. Early cluster expansion in these models is primarily driven by the expulsion of the remaining natal gas due to the massive-star feedback (stellar winds and supernovae). This suggests that a similar feedback-driven mechanism is likely to be responsible for the cluster structural evolution in the disc of M31.

In Fig. 2, we show the SC R_h as a function of galactocentric distance, R_{GC} . There is no clear dependence of SC sizes on the distance from the M31 centre. However, a very wide spread of SC sizes is prominent.

In the presentation, we will discuss the changes of the SC structure over time and within the M31 galaxy disc.

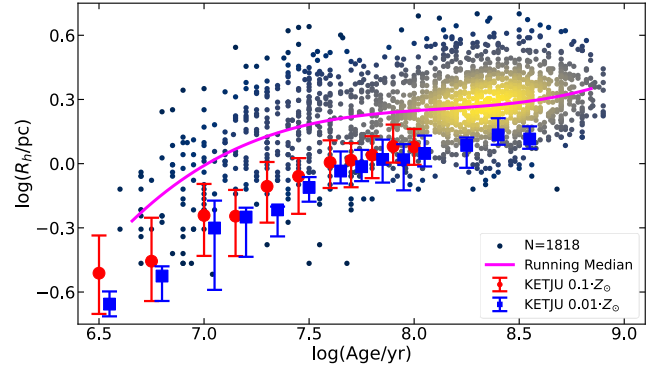


Fig. 1. SC half-light radii versus age. Blue markers and error-bars show median and spread (16-84 percentile range) of SC evolutionary models of 1 % solar metallicity [5]; red markers and error-bars show models of 10 % solar metallicity [N. Lahén, private commun.]. Blue markers are shifted by +0.05 along the X-axis for visual clarity.

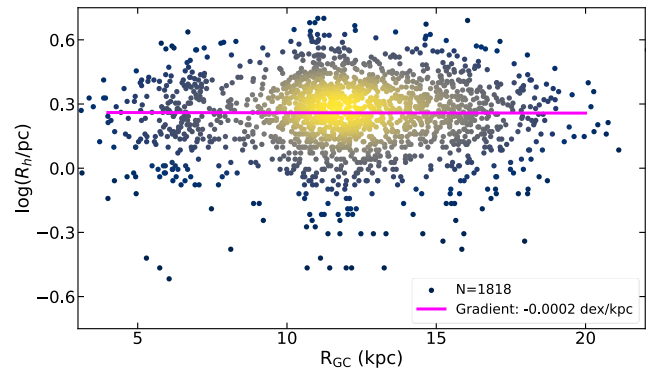


Fig. 2. SC half-light radii versus the M31 galactocentric distance.

References

1. C.J. Lada and E.A. Lada, *Ann. Rev. Astron. Astrophys.*, **41**, 57 (2003).
2. S.F. Portegies Zwart, S.L.W. McMillan, and M. Gieles, *Ann. Rev. Astron. Astrophys.*, **48**, 431 (2010).
3. J.J. Dalcanton, B.F. Williams, D. Lang, et al., *Astrophys. J. Supplement Series*, **200**, 18 (2012).
4. E. Kriščiūnas, R. Stonkutė, K. Daugevičius, et al., *Astron. Astrophys.*, submitted.
5. N. Lahén, A. Rantala, T. Naab, et al., *Mon. Not. R. Astron. Soc.*, **538**, 2129 (2025).

City-produced and transported black carbon: synergy of in-situ optical measurements and modeling

Agnė Minderytė¹, F. Moritz Hey^{2, 3}, Emeka A. Ugboma², Nikolaos Evangeliou⁴, Sabine Eckhardt⁴, Ignacio Pissó⁴, Steigvilė Byčenkienė¹ and I. S. Stachlewska²

1. Center for Physical Sciences and Technology, Department of Environmental Research
Saulėtekio av. 3, LT-10257 Vilnius, email: agne.minderyte@ftmc.lt
2. University of Warsaw (UW), Faculty of Physics, Warsaw, 02-093, Poland
3. Johannes Gutenberg University (JGU), Institute for Atmospheric Physics, Mainz, 55122, Germany
4. Norwegian Institute for Air Research (NILU), Department of Atmospheric and Climate Research (ATMOS), Kjeller, Norway

Urban areas experience elevated pollution levels due to local black carbon (BC) emissions, which contribute to increased pollution in surrounding regions through air mass long-range transport. Therefore, the need for investigating the BC sources and implications on radiative aerosol properties is crucial to have a more comprehensive understanding of aerosol dynamics in urban areas where the largest citizen population resides.

The study investigates BC source contribution and in situ measured aerosol optical characteristics, namely absorption, scattering and single scattering albedo (SSA) during the warm season of 2022 and the cold season of 2022/23 in two neighboring capitals, Vilnius and Warsaw. The measurement sites in urban (Warsaw) and urban background (Vilnius) environments were equipped with Aethalometers (AE33) and Nephelometers (TSI model 3563 in Vilnius site and Aurora 4000 in Warsaw site). BC source apportionment was performed using the Aethalometer model [1]. FLEXPART model was used to assess the effect of air mass long-range transport on local BC levels inside the investigated cities. A new method is explored for separating measured BC into city-produced BC and transported BC using FLEXPART model. Aerosol types were classified via the Absorption Ångström Exponent (AAE) and Scattering Ångström Exponent (SAE) optical division scheme suggested by Cappa et al. (2016) [2].

The two sites, despite being different in size and nature, exhibited similar source contributions during the warm season (the sources biomass burning (BB) and fossil fuel (FF) combustion as follows: 14% and 86% in Warsaw and 16% and 84% in Vilnius). However, during the cold season, significant use of coal burning (C) in Warsaw changed the distribution to 38% (BB+C) and 62% (FF) in Warsaw and 31% and 69% in Vilnius.

The optical aerosol classification based on AAE and SAE in Warsaw showed a higher presence of larger particle mixtures containing both BC and BrC in the cold season. Although BC dominated particles were still the most abundant for every month in the warm season (90%), as well as in the cold season (88%).

The impact of transported BC on the local BC levels in the cities was 47% and 64% in the cold season and 77% and 87% in the warm season for Warsaw and Vilnius, respectively. Thus, the approach of BC partitioning showed that in the cold season, the two cities experienced worse air quality due to increased transport of BC.

The study offers a more comprehensive understanding of prevailing BC sources, aerosol optical characteristics, and the impact of long-range transport on local BC levels in urban environments in the regions of Poland and Lithuania.

This work was supported by the joint Lithuanian-Polish research project DAINA-2 grant, the National Science Centre of Poland (Grant No. 2020/38/L/ST10/00480) and the Research Council of Lithuania (Grant No. S-LL-21-7). Measurements at the Warsaw site are supported by EC Horizon 2020, Gas No. 871115 (ACTRIS-IMP). Special thanks are given to the support of the Erasmus+ program of the European Union for financing the stay of Moritz Hey and Agnė Minderytė at UW.

References

- Sandradewi, J., Prévôt, A. S. H., Weingartner, E., Schmidhauser, R., Gysel, M., and Baltensperger, U. (2008) Atmos. Environ. 42, 101.
Cappa, C. D., Kolesar, K. R., Zhang, X., Atkinson, D. B., Pekour, M. S., Zaveri, R. A., Zelenyuk, A., Zhang, Q., (2016) Atmos. Chem. Phys. 16, 6511.

Tracing Photochemical Aging in Biomass Burning Aerosols Using Carbon Isotopes

Durre Nayab Habib¹, Andrius Garbaras¹, Ulrike Dusek², Agne Masalaite¹

1. Center for Physical Sciences and Technology, Department of Nuclear Research Saulėtekio av. 3, LT-10257
2. University of Groningen, Groningen, 9747 AG, The Netherlands, Durre.nayab@ftmc.lt

Aerosols from biomass burning are a major component of atmospheric particulate matter and play a critical role in air quality, climate, and health [1]. Understanding how these aerosols chemically evolve during atmospheric aging remains a key challenge, particularly regarding changes in their isotopic composition [2]. This study investigates the potential of carbon isotopic composition ($\delta^{13}\text{C}$) as a tracer for photochemical aging processes of biomass burning (BB) emissions.

Aerosol samples from the combustion of six different biomass fuels were collected. A high-flow sampler (DIGITEL DH-77) with a pre-separator (PM_{10}) was employed to collect biomass burning emission aerosols on Whatman QM-A pure quartz fiber filters. Isotopic composition of total carbon and organic carbon at three temperature steps (200 °C, 350 °C and 650 °C) was determined. Aging experiments were conducted in custom laboratory setups under either UV irradiation (308 nm) in an inert N_2 atmosphere or exposure to OH radicals generated via H_2O_2 photolysis, without UV exposure. In both cases, the aging process was carried out for 24 hours under nitrogen atmosphere.

OH-aged samples showed no significant isotopic shift. However, it could be seen for some samples that the total carbon masses in the 350 °C and 650 °C temperature steps only slightly deviated from the un-aged samples. For ash, there was an increase in total carbon mass measurements in OH aged sample (9.9 $\mu\text{g}/\text{cm}^2$ and 8.6 $\mu\text{g}/\text{cm}^2$) than the un-aged one (3.9 $\mu\text{g}/\text{cm}^2$ and 2.6 $\mu\text{g}/\text{cm}^2$) in 350 °C and 650 °C temperature steps. This is likely the result of an uneven distribution of the aerosol material on the filter. UV-aged samples exhibited consistent depletion in ^{13}C relative to un-aged samples, with a clear pattern across all fractions. Among the UV-aged samples, the products released in the 350 °C fraction were generally the most enriched in ^{13}C , as indicated by their higher $\delta^{13}\text{C}$ values compared to those from other temperature steps. For example, for wood pellets emissions, $\delta^{13}\text{C}_{\text{OC}}$ values for three temperature steps 200 °C, 350 °C and 650 °C are -25.3 ‰, -25.1 ‰ and -25.0 ‰ respectively. For un-aged samples, these values are -25.6 ‰, -25.7 ‰ and -25.4 ‰ for the three temperature steps 200 °C, 350 °C and 650 °C respectively. These results suggest that UV-induced processes may play a dominant role in atmospheric aerosol aging. $\delta^{13}\text{C}$ is a sensitive marker of photochemical aging. These findings highlight the value of isotopic analysis for linking controlled laboratory aging experiments with real atmospheric observations, providing a pathway toward improved source apportionment and assessment of aerosol impacts on climate.

References

1. Pöschl, Ulrich. "Atmospheric aerosols: composition, transformation, climate and health effects." *Angewandte Chemie International Edition* 44.46 (2005): 7520-7540.
2. Hu, W., Liu, D., Su, S., Ren, L., Ren, H., Wei, L., ... & Fu, P. (2021). Photochemical degradation of organic matter in the atmosphere. *Advanced Sustainable Systems*, 5(11), 2100027.

SOURCE APPORTIONMENT OF AEROSOL PARTICLES BY POSITIVE MATRIX FACTORIZATION IN URBAN BACKGROUND ENVIRONMENT (VILNIUS, LITHUANIA)

Viachaslau Alifirenka¹, Vitalij Kovalevskij¹, Mindaugas Gaspariunas¹, Mindaugas Bernatoniš², Steigvilė Byčėnienė¹

1. Center for Physical Sciences and Technology, Department of Environmental Studies, Saulėtekio av. 3, LT-10257 Vilnius, email: viachaslau.alifirenka@ftmc.lt

2. Environmental Protection Agency, A. Juozapavičiaus str. 9, LT-09311 Vilnius, Lithuania, email: aaa@gamta.lt

An aerosol is defined as a suspension of a liquid or solid particles suspended in a gas. Aerosols are a key contributor to environmental issues such as global warming, photochemical smog, and poor air quality. The health risks of aerosol exposure in urban areas pose a significant health concern. Awareness of the potential health impacts from aerosol anthropogenic sources particularly those associated with fine particles has increased only in recent years. The problem of environmental pollution in cities is relevant and the need to know the sources of pollution is a very important aspect for monitoring and reducing pollution [1].

The aim of this study was to determine the sources of aerosol particles using positive matrix factorization in an urban background environment. Measurements were performed from January 2 to December 21, 2019 at the urban background site located at the Vilnius. 100 samples of PM_{2.5} were collected on polytetrafluoroethylene filters and investigated by broad-beam particle-induced X-ray emission (PIXE) using 1.9 MeV protons. A proton beam, accelerated using a Tandetron 4110A ion accelerator and collimated to a diameter of 5 mm, was used to irradiate the samples. A single spectrum was measured for each PM_{2.5} sample, and the ppm (ng/cm³) levels were evaluated by assuming homogeneous deposition of PM on the filters. X-ray spectra were fitted using the GupixWin software package for quantitative elemental analysis. The NIST-2783 standart reference material (PM_{2.5} deposited on the filter) was used to calibrate the X-ray yield. Twenty one elements (Na, Mg, Al, Si, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, Br, Sr, Sn, Sb, Pb) were identified in the analysed samples. Figure 1 shows the distribution of concentrations of 21 identified elements and their presence in the factors.

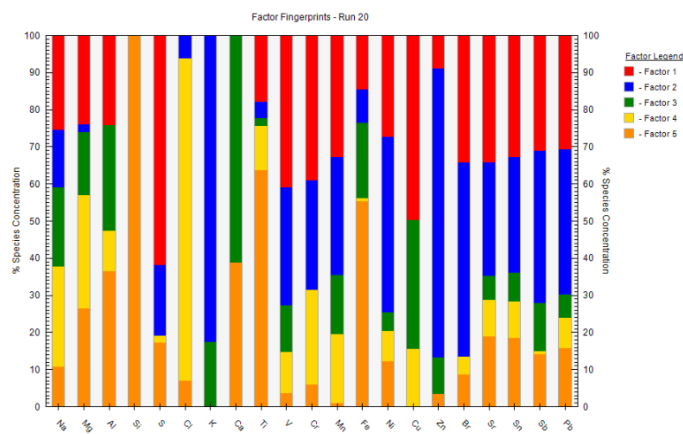


Fig.1. PM_{2.5} factors(sources) profile for Vilnius urban background area from 2 January to 21 December 2019.

Positive matrix factorization method was applied to assess the source apportionment of aerosol particles. The analysis revealed five factors(sources): factor 1 – Vehicle Emissions, factor 2 – Wood Burning, factor 3 – Soil Dust, factor 4 – Agricultural Activities, factor 5 – Crustal(Soil).

References

1. Aerosol science: Technology and applications. Ian Colbeck, Mihalis Lazaridis, 20

IMPACT OF THE PHYSICAL PROPERTIES OF LDPE MULCH FILMS ON PHOTOCATALYTIC DEGRADATION EFFICIENCY UNDER UV IRRADIATION

Sonata Pleskytė¹, Ieva Uogintė¹, Aušra Selskienė², Steigvilė Byčenkienė¹

1. Center for Physical Sciences and Technology, Department of Environmental Research
Saulėtekio av. 3, LT-10257 Vilnius, email: sonata.pleskyte@ftmc.lt
2. Center for Physical Sciences and Technology, Department of Characterization of Materials Structure
Saulėtekio av. 3, LT-10257 Vilnius

Plastic mulch films have been proven to increase nutrient use efficiency, soil water conservation, and provide effective weed and pest management in agroecosystems. Low-density polyethylene (LDPE) is one of the most widely used plastic types for producing mulch films, with more than 1.6 million tonnes of LDPE mulch films applied in agriculture worldwide, covering over 20 million hectares of farmlands [1]. In the natural environment, soil mulch films undergo various physical and chemical degradation processes, leading to breakdown into small fragments and the generation of excessive numbers of microplastics (< 5 mm). In particular, microplastics have been found to harm soil health and aquatic ecosystems, with a high potential to enter the food chain and pose risks to human health [2]. Agricultural films often become contaminated with soil, which makes them difficult to recycle. Thus, the advanced degradation technologies should be considered as one of the most promising tools to mitigate microplastic pollution.

This study aims to investigate the photocatalytic degradation of LDPE films, evaluating the impact of the physical properties of LDPE films on degradation efficiency. The photocatalytic test was conducted using LDPE mulch films in two sizes (1×1 mm and 3×3 mm) and two colors (black and transparent). As catalysts, Ag-TiO₂ nanomaterials were used. The photocatalytic

degradation tests were conducted in an aqueous medium under UV-A light irradiation for a set time period ranging from 60 to 960 minutes. The assessment of LDPE mulch films after photocatalytic degradation includes mass loss measurement, SEM imaging, and ATR-FTIR analysis.

The obtained results revealed that the size and color of LDPE mulch film influence photocatalytic degradation efficiency, with the highest mass loss of $9.88\% \pm 0.35\%$ found for black films (1 × 1 mm) after 960 minutes of exposure to UV light in the presence of Ag-TiO₂. The analysis of surface morphology has shown notable differences among the studied LDPE films. Specifically, black films have shown distinct alterations in the surface morphology, including the formation of flakes, wrinkles, cracks, cavities, and holes. The formation of oxygen-containing groups at region 1650-1850 cm⁻¹ was assigned to the carbonyl group and increased over the degradation time. The varying results among the studied LDPE films suggest that size and color play a crucial role in their interaction with UV-light and overall photocatalytic degradation efficiency. These results support the development of efficient advanced oxidation processes for managing agricultural plastic waste and global microplastic pollution.

References

1. K. Koskei et al., J Hazard Mater 414, (2021).
2. G. I. Senevirathne et al., Environmental Advances 20, (2025).

DEVELOPMENT OF THE NON-DESTRUCTIVE METHOD FOR THE DETERMINING SURFACE CONTAMINATION IN RADIOACTIVE WASTE

Kristina Mikalauskienė¹, Marina Konstantinova¹, Darius Germanas¹, Rita Plukienė¹, Elena Lagzdina¹, Artūras Plukis¹ ir Vidmantas Remeikis¹

1. Center for Physical Sciences and Technology, Department of Nuclear Research
Savanorių ave. 231, LT-02300 Vilnius, email: kristina.mikalauskiene@ftmc.lt

The growing need to reduce radioactive waste volumes or move to lower waste category by applying various decontamination techniques challenges characterization of radioactive waste to distinguish between internal activity or surface contamination that can be removed.

The investigated non-destructive method for determining radioactive waste contamination is based on gamma-ray spectrometric analysis. The method uses the Compton-to-peak ratios for estimate the attenuation of photons due absorption and scattering processes when gamma rays pass through samples of metal or concrete waste. By analyzing the ratios of the Compton edge or backscattering regions of spectra to the photopeak region, it is possible to determine whether radionuclide contamination is on surface, at a shallow depth, or deeper [1]. This is important for the reliable assessment of waste, where knowledge of the depth of contamination is crucial for decisions on long-term storage or recycling processes after the decommissioning of nuclear power plant [2].

We performed investigations with laboratory-made samples of ^{137}Cs and ^{60}Co point sources, imitating real radioactive waste using a high-purity germanium (HPGe) detector and a portable cerium bromide (CeBr_3) scintillation detector. The mentioned radionuclides in the samples were distributed either as surface contamination or as heterogeneously located activity within the sample volume.

The efficiency calibrations of both detectors were performed for the standard measurement geometry using certified reference sources of ^{137}Cs and ^{60}Co [3]. additionally, in case with CeBr_3 detector, energy scale drift caused by temperature fluctuations in the room or outside environment was taken into account by correcting the energy calibration, which is particularly important for longer measurement durations.

Accurate MCNP6 simulations were performed for each case for validation purposes. A comparison between the simulated and experimental gamma spectra shows good agreement for both cases obtained from ^{60}Co source on surface and at 1 cm depth in steel sample (see Figure 1), using a CeBr_3 detector. Similar consistency is also observed in the spectra obtained using HPGe detector. Furthermore, the 1σ agreement was obtained for the ratios of the Compton edge-to-the photopeak or Compton backscatter-to-the photopeak obtained from spectra in both detectors.

The results indicate that the analysis of gamma-ray intensity and the Compton-to-peak ratios, combined with simulations, can be used to determine the distribution of unknown ^{137}Cs and ^{60}Co sources in metal/concrete waste. A portable CeBr_3 detector, despite having lower resolution than HPGe, is suitable

for distinguishing between surface and depth contamination. This method can be effectively applied not only for characterization of unknown sources, but also for radioactive waste sorting and for the improvement of nuclide vectors at final disposal sites.

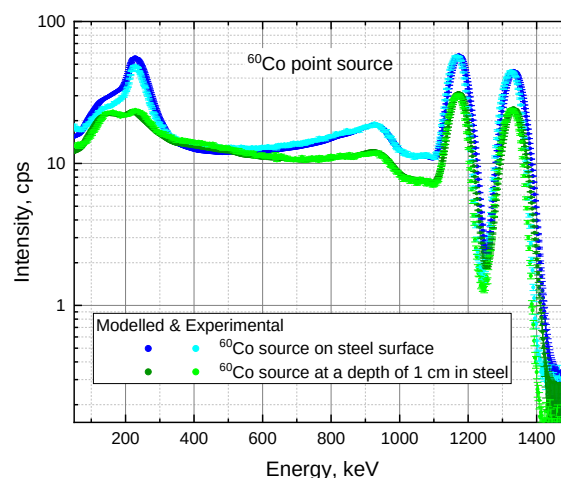


Fig.1. Comparison of MCNP simulated and experimental gamma spectra obtained with a CeBr_3 detector under outdoor conditions for ^{60}Co surface and ^{60}Co source at 1 cm depth in steel sample.

References

1. K. Mikalauskienė et al., Assessment of Compton/photopeak ratio for various thickness metal shielding, Proc. of Int. Conf. "Medical Physics in the Baltic States 2023", 09-11 November, 2023, Kaunas, Lithuania.
2. V. Remeikis, J. Grinevičiūtė, G. Duškesas, L. Juodis, R. Plukienė, A. Plukis, Nucl Eng Des, 239(4), 813-818 (2021).
3. M. Konstantinova, D. Germanas, A. Gudelis, A. Plukis, Lith. J. Phys., 61, 1, 66-73.

Development of modified graphene oxide nanocomposite for the removal of nanoplastics from fresh water

Mahrosh Javed¹, Galina Lujanienė¹, Sergej Šemčuk¹, Vidas Pakštas¹, Aušra Selskienė¹,

Audrius Drabavičius¹, Martynas Talaikis¹

1. Center for Physical Sciences and Technology, Department of Environmental Research

Saulėtekio av. 3, LT-10257 Vilnius, email: mahrosh.javed@ftmc.lt

Over the past decade, the overuse of plastics in all areas of society has led to widespread plastic pollution of water, air, and soil. These overused plastics gradually break down into small pieces and form micro- (<5mm) and nanoplastics (<1μm-100nm). These micro- and nanoplastics are difficult to degrade, and recent research has reported their toxic effects on human health [1]. Water is a vital component of all life, so its purity is an urgent need for the substance of life. As the increasing pollution of the environment by plastics jeopardises water quality, researchers need to look for environmentally friendly and sustainable ways to treat water. Therefore, this study focuses on the development of modified graphene oxide nanocomposites to remove four types of nanoplastics from freshwater. Graphene oxide is a good adsorbent due to its many functional groups and hydrophilicity.

To improve the adsorption capacity, chitosan and cellulose [2] were used to modify graphene oxide [3]. These nanocomposites were synthesised by chemical crosslinking with glutaraldehyde. After synthesis, these nanocomposites were characterised by SEM, XRD, and FT-IR. Nanoplastics of polystyrene (PS), polyethylene (PE), polyethylene terephthalate (PET), and polypropylene (PP) were synthesised by nanoprecipitation. These nanoplastics were characterised by TEM and FT-IR spectroscopy. These adsorbents were used for the removal of the prepared NPs from aqueous media. The adsorption study focused on a batch experiment to measure pH, adsorbent dosage, contact time, initial concentration of the nanoplastic, and temperature. The adsorbents were then re-characterised and compared to their original SEM, XRD and FT-IR data. The results obtained are used for kinetic, isothermal, and thermodynamic studies to determine the removal efficiency and adsorption capacity. Below are the results of the SEM studies for Polystyrene nanoplastics (PS-NPs), Polyethylene nanoplastics (PE-NPs), Polypropylene nanoplastics (PP-NPs), and Polyethylene terephthalate nanoplastics (PET-NPs) in Fig. 1.

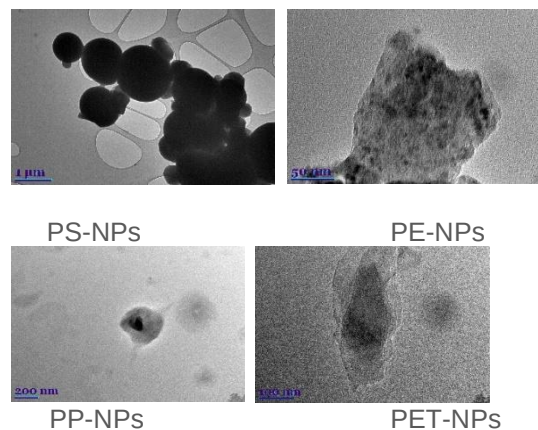


Fig. 1. TEM images of PS-NPs, PE-NPs, PP-NPs and PET-NPs.

References

1. Javed, M. and G. Lujanienė, Nanoplastics in aquatic systems: challenges and advances in adsorptive removal technologies. *Frontiers in Water*, 2025. 7: p. 1611558.
2. Sun, J., et al., Effective removal of nanoplastics from water by cellulose/MgAl layered double hydroxides composite beads. *Carbohydrate Polymers*, 2022. 298: p. 120059.
3. Li, Z., et al., Multifunctional sodium alginate/chitosan-modified graphene oxide reinforced membrane for simultaneous removal of nanoplastics, emulsified oil, and dyes in water. *International Journal of Biological Macromolecules*, 2023. 245: p. 125524.

DEVELOPMENT OF MAGNETIC BUCKWHEAT HULL- Fe_3O_4 NANOCOMPOSITE FOR BIOSORPTION OF Pb(II) , Cd(II) , AND Cr(III) FROM MIXED HEAVY METAL WASTEWATER

Tayyab Tahir¹, Rūta Druteikienė¹, Zita Žukauskaitė¹, Jūratė Vaičiūnienė²

1. Center for Physical Sciences and Technology, Department of Nuclear Research
Savanorių ave. 231, LT-02300 Vilnius, email: tayyab.tahir@ftmc.lt
2. Center for Physical Sciences and Technology, Department of Catalysis
Saulėtekio av. 3, LT-10257 Vilnius,

The large scale release of heavy metals from several industrial sources is placing significant stress on the environment and has become a major concern. Because of their persistent nature, these metals accumulate in ecosystems, negatively impacting living organisms. Particularly hazardous heavy metals, even at very low concentrations, include cadmium, chromium, mercury, nickel and lead [1]. Many efforts have previously been made to address environmental pollution. The removal of heavy metal ions from wastewater can be attained through a various array of techniques, including ion exchange, oxidation–reduction, precipitation, evaporation, filtration, reverse solvent extraction and osmosis. However, these methods have several drawbacks, including extreme consumption of chemicals and energy, incomplete metal binding, and the production of toxic sediments and waste products. Heavy metal pollution in water remains a significant challenge, for which biosorption represents a promising solution [2].

The application of nano-adsorbents for removing heavy metal contaminants has demonstrated considerable promise owing to their unique properties, such as large surface area, excellent reusability, high thermal stability, enhanced regeneration efficiency, small particle size, and magnetic behavior. Among the nanoparticles, Fe_3O_4 -based magnetic adsorbents have attracted worldwide attention because of their ease of separation [3].

In this study, buckwheat hull- Fe_3O_4 (BWH- Fe_3O_4) nanocomposite was synthesized and assessed as an efficient biosorbent, exhibiting easy magnetic separation and high selectivity for heavy-metal removal. The material was characterized before and after sorption using FT-IR, SEM, EDX, and point of zero charge (pH_{pzc}) analyses.

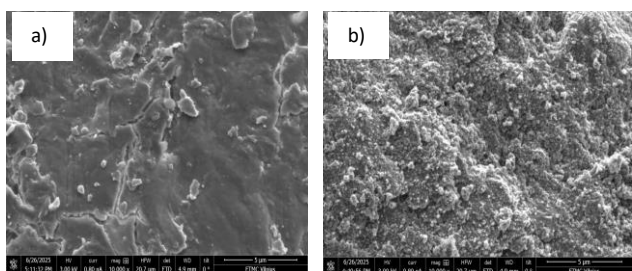


Fig. 1. SEM images of (a) buckwheat hull (b) buckwheat hull- Fe_3O_4 nanocomposites.

Its removal efficiency and sorption capacity were evaluated through batch experiments under varying operational parameters, including solution pH, biosorbent dose, contact time, initial metal ions

concentration, temperature, and agitation rate. Furthermore, the sorption kinetics, equilibrium isotherms, and thermodynamic studies were systematically investigated to elucidate the underlying mechanisms.

The biosorption experiments exhibited that at optimal conditions for Pb(II) , Cd(II) and Cr(III) at pH 6, initial concentration of each metal ions 5 mg L^{-1} , contact time 180 min, sorbent dosage 0.1 g , temperature 298 K , BWH- Fe_3O_4 nanocomposites has high sorption efficiency of about 97% for Pb(II) , 76% for Cd(II) and 89% for Cr(III) . Kinetics models (as pseudo-first-order, pseudo-second-order, intraparticle diffusion and Elovich) were applied in the study of sorption data. The pseudo-second-order kinetic model yielded higher agreement with experimental results in comparison to the pseudo-first-order kinetic model due to the higher values of $R^2_{\text{Pb(II)}}=0.999$, $R^2_{\text{Cd(II)}}=0.999$ and $R^2_{\text{Cr(III)}}=0.999$. The obtained R_L value of Pb(II) , Cd(II) and Cr(III) sorption, which ranged from 0.05 to 0.33, 0.09 to 0.51 and 0.03 to 0.26, respectively indicates that metal ions adsorption was favorable on the BWH- Fe_3O_4 nanocomposites's surface. The thermodynamic parameters (i.e.: entropy, Gibbs free energy, and enthalpy) show that removal of Pb(II) by buckwheat hulls is an endothermic and spontaneous process. Meanwhile, Cd(II) and Cr(III) sorption is an exothermic and non-spontaneous process.

References

1. M.Priyadarshane and S.Das, Chemosphere 368, 143681 (2024).
2. H.Şensöz and R.Donat, Mater. Sci. Eng. B 314, 118067 (2025).
3. M.Saberi-Zare and M.A.Bodaghifard, Int. J. Biol. Macromol. 296, 139794 (2025).

CFD Modeling and Optimization of Forced-Air Cooling in Indoor LiFePO₄ Battery Energy Storage Cabinets

Gediminas Skarbalius¹, Mantas Mackelis¹, Artūras Baronas², Saulius Gudžius²

1. Laboratory of Heat-Equipment Research and Testing, Lithuanian Energy Institute, Breslaujos st. 3, LT-44403 Kaunas, Lithuania, email: Gediminas.skarbalius@lei.lt
2. Department of Electrical and Power Systems, Kaunas University of Technology, K. Donelaičio st. 73, LT-44249, Kaunas, Lithuania

Intermittent output from renewable sources (solar PV, wind) challenges grid stability, necessitating large-scale energy storage [1,2]. For indoor utility-scale deployments, lithium-ion battery cabinets—valued for high energy density, fast response, and modularity—are commonly managed with forced-air cooling [3,7]. Battery cell performance and life are temperature-dependent: elevated or non-uniform temperatures accelerate capacity fade, hotspots, and uneven ageing, undermining reliability and safety [4,5]. Thus, robust thermal management of air-cooled cabinets is essential to maintain safe, uniform operating temperatures [3,6,7].

In this study, we developed a universal three-dimensional Computational Fluid Dynamics (CFD) framework for battery energy storage systems that resolves fluid flow and conjugate heat transfer between solid components and the surrounding air. We applied the model to a representative indoor storage cabinet comprising ten 16-cell LiFePO₄ modules with forced-air cooling. The verification case was simulated under typical operating/cooling conditions with bulk inlet velocity ≈ 1 m/s and total cell heat generation of 640 W (4 W per cell). From the simulations results, temperature fields, thermal gradients, and flow distribution was assessed.

The simulation results given in Figure 1a) show that the air speed is highest around the lower modules, but as the flow rises, it spreads more evenly around the battery modules. The lowest velocities occur in the gaps between modules on adjacent shelves. Streamlines reveal that vortices form downstream of the modules, which can reduce heat removal from those regions. This is followed to slight air temperature raises of the ambient air as seen in Figure 1b).

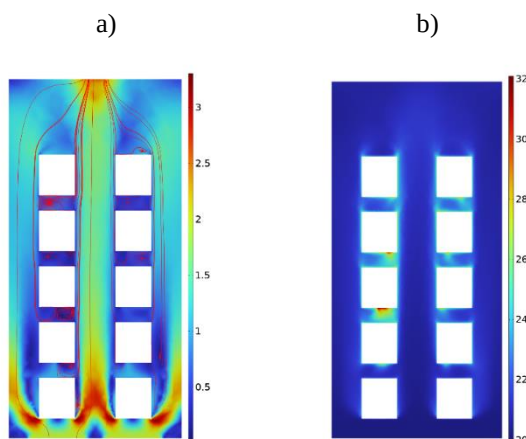


Fig. 1. a) Air velocity field with streamlines (m/s) and b) air temperature (°C) in the plane at through the module centre.

The cell surface temperature plot given in Figure 2 indicates that cell surface temperature increases with the modules' distance from the air inlet zone. The highest module temperature in the simulation was recorded at the top of the modules in row 4; under the chosen operating and cooling conditions this maximum surface temperature was 43.4 °C. Also, the higher temperatures develop in the middle and rear parts of the modules. Conversely, the top-row modules are

slightly cooler than the row beneath them because they have no upper neighbouring modules to impede airflow or trap heat.

Future work will update and validate the model against experimental measurements once the prototype is produced. Following validation, the model will be used to optimize cooling flow regimes to maintain uniform cell temperatures and minimize auxiliary energy consumption. Once the model is validated, it could be used to estimate the performance of various types of battery storage systems and aid their development.

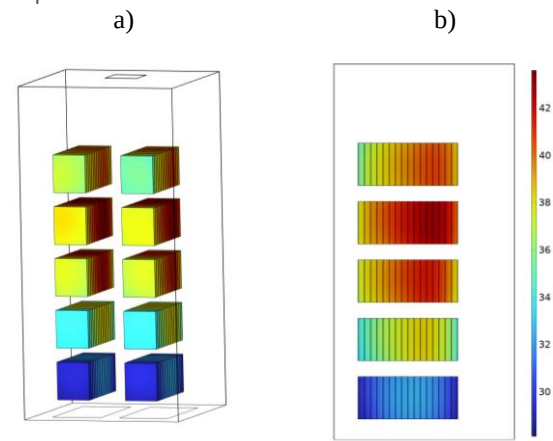


Fig. 2. Cell surface temperature distribution: (a) front view and (b) side view from the right.

ACKNOWLEDGMENT

This research was funded by „New Generation Lithuania” (NKL) plan, financed by the European Union's Economic Recovery and Resilience Facility (RRF) as part of the execution of the “Mission-driven Implementation of Science and Innovation Programmes” project (No. 02-002-P-0001).

References:

1. P. Cosgrove, T. Roulstone, and S. Zachary, “Intermittency and periodicity in net-zero renewable energy systems with storage,” *Renewable Energy*.
2. F. H. Malik, G. A. Hussain, Y. M. S. Alsmadi, Z. M. Haider, W. Mansoor, and M. Lehtonen, “Integrating energy storage technologies with renewable energy sources: A pathway toward sustainable power grids,” *Sustainability*.
3. Y. Wang, X. Yin, X. Li, H. Li, S. Liu, X. Zhu, and X. Ma, “Minimum air cooling requirements for different lithium-ion battery operating statuses,” *ASME Journal of Heat Transfer*.
4. S. Li, C. Zhang, Y. Zhao, G. J. Offer, and M. Marinescu, “Effect of thermal gradients on inhomogeneous degradation in lithium-ion batteries,” *Communications Engineering*, vol. 2, art. 74, 2023.
5. W. Shen, N. Wang, J. Zhang, F. Wang, and G. Zhang, “Heat generation and degradation mechanism of lithium-ion batteries during high-temperature aging,” *ACS Omega*.
6. G. Zhao, X. Wang, M. Negnevitsky, and H. Zhang, “A review of air-cooling battery thermal management systems for electric and hybrid electric vehicles,” *Journal of Power Sources*.
7. Y. Lin, Y.-W. Chen, and J.-T. Yang, “Optimized thermal management of a battery energy-storage system (BESS) inspired by air-cooling inefficiency factor of data centers,” *International Journal of Heat and Mass Transfer*.

P1 did not attend.

Additive Manufacturing Approach for the Development of Piezoelectric Polymer–Ceramic Composites

Bilal Islam¹, Karolis Bendiniskis¹, Nabeel Maqsood¹, Genrik Mordas¹

Center for Physical Sciences and Technology, Department of Laser Technology
Savanorių pr. 231, LT-02300 Vilnius, Lithuania, email: bilal.islam@ftmc.lt

Limitations of conventional fabrication methods for complex and customized micro-architectures are constraining the miniaturization, functionality, and performance of the latest generation of piezoelectric devices, especially in applications such as energy harvesting and sensing. Recent studies have demonstrated that additive manufacturing techniques enable the creation of advanced polymer–ceramic composites with tailored geometries and enhanced functionalities [1].

This work introduces a novel approach based on Stereolithography (SLA) additive manufacturing for the fabrication of functional polymer–ceramic composite structures by incorporating high-stiffness Silicon Carbide (SiC) microparticles into a photo-curable epoxy resin base. The main objective was to maximize the SiC filler loading while maintaining printable rheology and significantly enhancing the mechanical and dielectric performance of the composite—key parameters for efficient piezoelectric response.

Stable, low-viscosity suspensions suitable for SLA printing were successfully produced, exhibiting uniform dispersion of SiC particles up to 0, 1, 2.5 and 5 wt%. SLA parameters i.e, normal exposure time ~3–5 s, number of layers 6 and bottom exposure was kept constant ~20 s. The printed specimens demonstrated a 25 and 35% increase in hardness and Young's modulus, resulting in improved structural integrity and acoustic impedance necessary for stress transfer in sensing applications. The high dielectric constant of SiC contributed to an increased overall relative permittivity (ϵ_r) of the composite, consistent with previous findings on epoxy/SiC systems [2]. This enhancement allowed a reduction in the required electric field strength and promoted more complete and uniform polarization of the active piezoelectric phase.

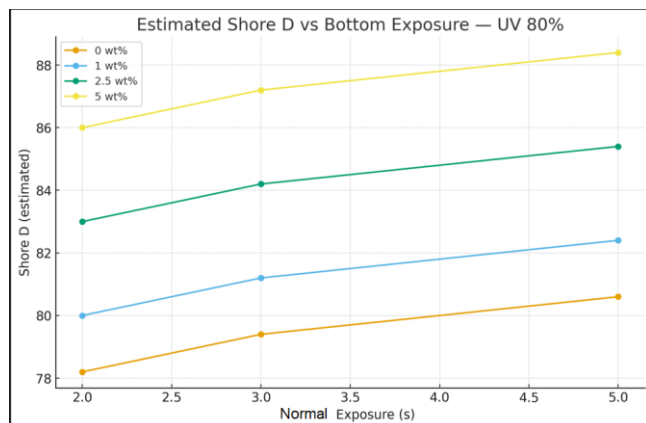


Figure 1. Shore D dependence on the normal exposure time

Leveraging the design freedom of SLA, complex 1–3 lattice structures were more crystalline with increment

in loading percentage and exposure time (as shown in Figure 2) and printed, exhibiting higher electromechanical coupling coefficients (k) compared to conventionally cast composites which is validated by increase in modulus values. Increasing modulus and hardness also means increase in crosslinking density. Hence, as a consequence electromechanical coupling coefficients will also enhance positively.

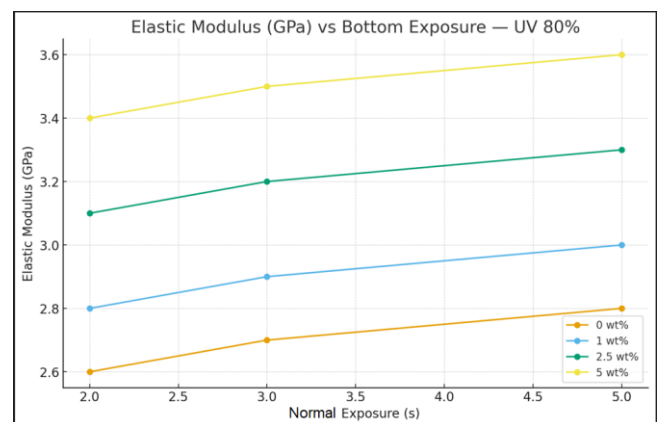


Figure 2. Normal exposure time plotted vs Elastic modulus.

This study demonstrates that mechanically robust, custom-geometry piezoelectric components can be rapidly prototyped using an SLA-based platform. Such a scalable and versatile fabrication route opens new possibilities for the development of high-performance SiC-reinforced sensors and micro-actuators for advanced piezoelectric applications.

References

1. Y. Wang, Z. Chen, Z. Zhang, Z., and Y. Li, Compos. Part B: Eng. **224**, 109150 (2021).
2. H. Gong, E. Budianto, and D. Li, J. Mater. Sci: Mater. Electron., **31**, 10403–10412.

IMPACT OF THE PROTEIN ENVIRONMENT ON THE EXCITED STATES OF THE PIGMENTS IN PHOTOSYNTHETIC COMPLEXES

Gabrielė Rankelytė¹

¹Center for Physical Sciences and Technology, Department of Molecular Compound Physics
Saulėtekio av. 3, LT-10257 Vilnius, email: vardas.pavarde@ftmc.lt

The most efficient organisms that carry out photosynthetic reactions are higher plants (or land plants). Inside the thylakoid membrane of chloroplasts there are two systems that perform photosynthesis: Photosystem I and Photosystem II. Photosystem I (PSI) is the most efficient light-to-energy conversion apparatus where almost all light, absorbed by the light harvesting antenna LHCI, is converted to chemical energy (1).

In plants, light harvesting antenna of Photosystem I is composed of four species of LHCI complexes. They all have very similar structure (see Fig. 1, where geometry of Lhcas is compared by mapping the subcomplex structures on top of each other); however, their spectral properties are different. The main difference, observed in the fluorescence spectra of the reconstituted Lhca1-Lhca4 subcomplexes (2), is the absence of the red-shifted peak (~730 nm) in two out of four subcomplexes. The most red-shifted peak is observed in the fluorescence spectrum of Lhca4. Despite the differences, all four Lhca subcomplexes have a peak at ~680 nm.

The excitation dynamics in LHCI antenna are highly affected by the charge-transfer (CT) states that occur between the pigments (two or more pigments: chlorophylls or/and carotenoids). Known charge-transfer sites in LHCI do not completely explain the spectral properties of this antenna nor do they describe the energy pathway from the antenna to the Photosystem I core well, suggesting the presence of more CT states. The energy of these states is affected by the surrounding environment (pigments and protein).

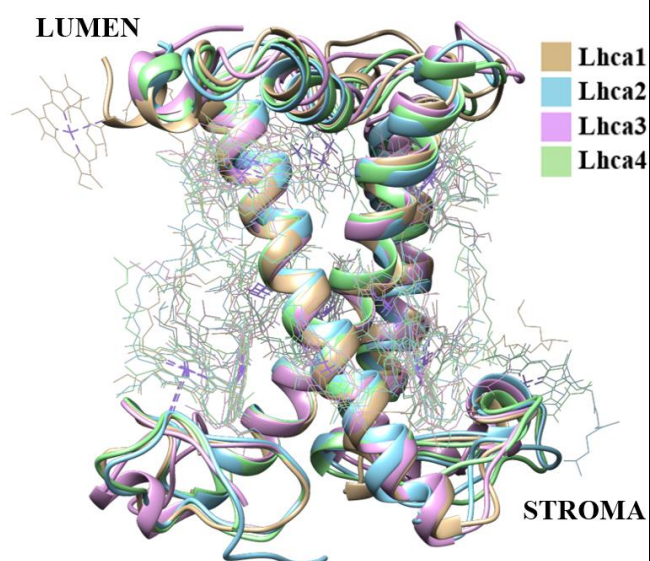


Fig. 1. Matched Lhca1-Lhca4 sub-complexes of LHCI (PDB ID: 5L8R, chains 1-4).

In our work, we have investigated the crystal

structure of LHCI antenna of PSI complex, available at Protein Data Bank (PDB ID: 5L8R) (3). Properties of the excited states of the pigments in vacuum were calculated using "VU HPC" Saulėtekis supercomputer. The charge-transfer state has an explicit property which makes it simple to find: the charges are distributed among the participating pigment monomers (easy to notice when looking into the sum of Mulliken partial charges for the monomers). Meanwhile, ordinary excited states do not possess this property, and the pigments carry neutral charge.

To evaluate the environmental energy shift, we have used two different methods. Charge-density coupling method (4) was used to explicitly evaluate excited state energy shifts, caused by the electrostatic environment, as a separate quantity (TD-DFT + CDC), after performing TD-DFT *in vacuo*. Another method (TD-DFT + Charge), instead of conducting QC calculations in vacuum, performs TD-DFT directly inside the charge field. The results of the TD-DFT + CDC method were compared to the results of TD-DFT + Charge (see energy comparison of low energy CT states in Fig. 2). Our findings demonstrate the sensitivity of pigment excited state properties to the selected QC method as well as it provides the pros and cons to the methods themselves in terms of the computational time and compatibility with the CT state calculations.

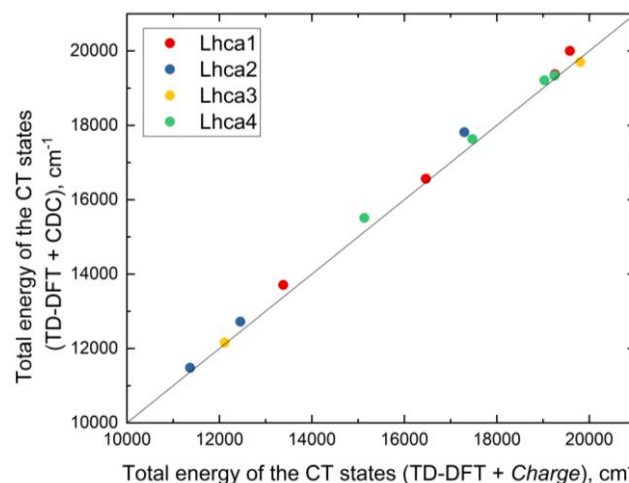


Fig. 1. Low-energy CT state comparison between TD-DFT + CDC and TD-DFT + Charge methods.

References

1. R. Croce, H. van Amerongen, Photosynth. Res., **116**, 153-166 (2013).
2. E. Wientjes, I. H. Van Stokkum, H. Van Amerongen, and R. Croce, Biophys. J. **100**, 1372-1380 (2011).
3. Y. Mazor, A. Borovikova, I. Caspy and N. Nelson, Nat. Plants., **3**, 17014-17014 (2017).
4. T. Renger, F. Müh, Phys. Chem. Chem. Phys., **15**, 3348-3371 (2013).

MOLECULARLY IMPRINTED POLYMERS AS SELECTIVE RECOGNITION ELEMENTS FOR GERANIOL DETECTION

Greta Kasputė¹, Urtė Prentice¹

¹Center for Physical Sciences and Technology, Department of Nanotechnology
Saulėtekio av. 3, LT-10257 Vilnius, email: greta.kaspute@ftmc.lt

Molecularly imprinted polymers (MIPs) have attracted considerable attention for their ability to selectively recognize target analytes within complex matrices. Constructing an effective and stable MIP requires assessing the likelihood of analyte adsorption on the sensor surface. Molecular imprinting technology (MIT) provides a synthetic route to durable recognition materials that mimic natural receptors and antibodies. The process involves forming a polymer matrix around a template molecule, which is subsequently removed to create highly specific binding sites. These recognition sites interact with the target through forces such as hydrogen bonding, dipole–dipole interactions, and ionic attractions [1,2].

Geraniol (C₁₀H₁₈O; 3,7-dimethyl-2,6-octadien-1-ol) is an acyclic monoterpenoid alcohol, belonging to the family of isoprenoids [3]. Structurally, it contains two conjugated double bonds and a primary alcohol group, which confer both reactivity and versatility for chemical transformations. From a chemical standpoint, geraniol serves as an important biosynthetic intermediate in the mevalonate and methylerythritol phosphate (MEP) pathways that generate terpenes and terpenoids [3]. It is a precursor for the biosynthesis of several higher-order terpenes, such as citronellol, nerol, geranyl esters, and ionones, which are of interest in both natural product chemistry and synthetic organic chemistry. Geraniol is also widely employed as a starting material in synthetic chemistry. Its double bonds make it a useful substrate for oxidation, hydrogenation, epoxidation, and cyclization reactions [3].

In this work, we developed a MIP-based quartz crystal microbalance (QCM) sensor prototype for the selective detection of geraniol. Pyrrole-based MIP films were electropolymerized on gold electrodes, and characterization with cyclic voltammetry and QCM confirmed specific geraniol adsorption. A comparative study of single- and double-layer MIP designs revealed that the double-layer configuration enhanced both stability and selectivity. In contrast, non-imprinted polymer (NIP) controls showed negligible responses, confirming the effectiveness of the imprinting process.

The sensor exhibited concentration-dependent behavior, with strong and partially irreversible adsorption at low concentrations, indicating high affinity binding sites for geraniol. Beyond selective recognition, the findings suggest a potential dual functionality of MIP-based systems, serving not only as analytical sensors but also as platforms for purification or controlled release. Overall, this study demonstrates a promising pathway toward next-generation MIP technologies with applications in essential oil analysis, environmental monitoring, and biomedical fields.

I want to express my gratitude to Dr. Deivis Plaušinitis for his valuable contributions and insightful guidance throughout this research.

References

1. Vasapollo G, Sole RD, Mergola L, Lazzoi MR, Scardino A, Scorrano S, et al. Molecularly Imprinted Polymers: Present and Future Prospective. *International Journal of Molecular Sciences*. 2011;12(9):5908.
2. Kaspute G, Ramanavicius A, Prentice U. Molecular Imprinting Technology for Advanced Delivery of Essential Oils. *Polymers*. 2024 Jan;16(17):2441.
3. Chen W, Viljoen AM. Geraniol — A review of a commercially important fragrance material. *South African Journal of Botany*. 2010 Oct 1;76(4):643–51.

Systematic Study of Sulfuric Acid Anodization Parameters for Satellite-Grade Aluminum Alloys

Paulius Baronas¹, Tadas Matijošius², Artūras Suchodolskis³, Inga Morkvėnaitė-Vilkončienė¹

¹Center for Physical Sciences and Technology, Department of Nanotechnology
Saulėtekio av. 3, LT-10257 Vilnius. Email: paulius.baronas@ftmc.lt

²Center for Physical Sciences and Technology, Department of Chemical Engineering and Technology
Saulėtekio av. 3, LT-10257 Vilnius

³Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius

Anodized aluminum is widely used in space applications, due to excellent strength to weight ratio, cold welding and corrosion resistance, desirable thermo-optical properties. Previous investigations into the performance of anodized aluminum coatings under high temperature and vacuum did not fully address the combined influence of alloy composition, heat treatment, porosity, layer thickness, and sealing method. Earlier studies, including those by NASA and Goueffon et al. [1–6], identified cracking and flaking in anodic films exposed to thermal and vacuum environments but were limited to single aluminum grades, primarily dyed coatings, and lacked systematic analysis of porosity and sealing effects. Therefore, this work aims to systematically investigate anodization process parameters which influence anodic coating characteristics relevant in space applications.

In this study, anodic coatings were produced on multiple aluminum grades and tempers to evaluate their surface roughness and solar absorptance values dependency based on anodization process parameters. The investigated parameters included alloy type, temper, anodization bath temperature and sulfuric acid concentration (influencing porosity), anodic layer thickness, and sealing method. The relationships between these variables and coating performance were established.

After anodization, samples underwent optical inspections with digital microscope, peel testing, surface roughness measurements. Furthermore, solar absorptance measurements in 250nm-2500nm wavelength range were performed to assess optical property changes relevant to thermal control.

Obtained results demonstrated clear correlations between anodizing parameters and certain coating characteristics. The measured surface roughness (R_a) values are higher, for samples with more visual defects. Furthermore, measured R_a shows inverse correlation with used sulfuric acid concentration. Higher thickness samples show higher solar absorptance. Non-sealed samples have higher absorptance than sealed. 6082 grade aluminums have highest absorptance as a grade group, however 7075 grade T651 temper has highest absorptance overall.

Upon full study completion, the most optimal anodization parameters, which result in most relevant characteristics will be proposed for use in space applications.

References

1. Goueffon, Y.; Arurault, L.; Fontorbes, S.; Mabru, C.; Tonon, C.; Guigue, P. Chemical Characteristics, Mechanical and Thermo-Optical Properties of Black Anodic Films Prepared on 7175 Aluminium Alloy for Space Applications. *Mater Chem Phys* 2010, 120, 636–642.
2. Goueffon, Y.; Aldebert, G.; Mabru, C.; Arurault, L.; Tonon, C.; Guigue, P. Flaking of Black Anodic Films in Space Environment: Ageing and Numerical Simulation. *Mechanics of Materials* 2012, 45, 72–82.
3. He, C.C. Preventing Cracking of Anodized Coatings; Goddard Space Flight Center, National Aeronautics and Space Administration, 1995; Vol. 104622.
4. Goueffon, Y.; Arurault, L.; Mabru, C.; Tonon, C.; Guigue, P. Black Anodic Coatings for Space Applications: Study of the Process Parameters, Characteristics and Mechanical Properties. *J Mater Process Technol* 2009, 209, 5145–5151, doi:10.1016/j.jmatprotec.2009.02.013.
5. Goueffon, Y.; Mabru, C.; Labarrère, M.; Arurault, L.; Tonon, C.; Guigue, P. Investigations into the Coefficient of Thermal Expansion of Porous Films Prepared on AA7175 T7351 by Anodizing in Sulphuric Acid Electrolyte. *Surf Coat Technol* 2010, 205, 2643–2648, doi:10.1016/j.surfcoat.2010.10.026.
6. He, C.C.; Heslin, T.M.; Goddard, N. Preventing Cracking of Anodized Coatings (NASA-TM-104622) PREVENTING CRACKING OF ANODIZED COATINGS; 1995;

Improving membrane coating approaches to promote cell adhesion in two-channel microphysiological systems

Kamilė Kasperavičiūtė¹, Eivydas Andriukonis¹, Arūnas Stirkė¹, Wanessa Melo¹

¹Center for Physical Sciences and Technology, Department of Functional Materials and Electronics
Saulėtekio av. 3, LT-10257 Vilnius, email: kamile.kasperaviciute@ftmc.lt

Microphysiological systems, particularly organ-on-chip platforms, are increasingly recognized for their ability to replicate tissue barriers and dynamic cellular interactions more effectively than conventional culture models [1]. Two-channel architectures separated by porous membranes are widely applied to mimic epithelial and endothelial interfaces, as they allow for co-culture and bidirectional communication, however their performance often depends on achieving sufficient cell adhesion on synthetic membranes [2]. Limited adhesion reduces the physiological relevance and reproducibility of such models, highlighting the need for improved surface modification strategies.

In this work, porous membranes were modified through a sequential coating approach using polyethyleneimine (PEI 600) followed by dopamine hydrochloride, and compared to untreated controls. The modified membranes were characterized prior to integration into two-channel devices to assess their suitability for

supporting cell culture. Surface analyses by FTIR, Raman spectroscopy, and AFM confirmed chemical and topographical alterations induced by the treatment. Microscopy observations further indicated enhanced cellular adhesion on modified membranes compared to unmodified ones.

These results demonstrate that combining polymeric and bio-inspired coatings can improve membrane properties, thereby increasing the robustness and reproducibility of microphysiological barrier models.

References

1. Moon, H.-R., Surianarayanan, N., Singh, T., & Han, B., *Biomicrofluidics*, 17(6), 061504 (2023).
2. Chen, S., Xue, J., Hu, J., Ding, Q., Zhou, L., Feng, S., Cui, Y., Lü, S., & Long, M., *Acta Mech. Sin.*, 36(3), 754–767 (2020).

Development of a Biocompatible Polymer-Based Drug Delivery System

Felix Lücke¹, Elena Nedzinskaitė¹, Šarūnas Žukauskas¹;

¹Center for Physical Sciences and Technology, Department of Nano Technologies
Saulėtekio av. 3, LT-10257 Vilnius, email: felix.luecke@ftmc.lt

The most common drug delivery methods like oral or intravenous delivery often suffer from low bioavailability, low patient compliance and a limited targeting ability. Furthermore, many drug types (e.g.: peptides, genes, and small molecules) are challenged by poor solubility, lipophilicity, enzymatic degradation, low absorption inside the body and premature activation.[1, 2] Drug delivery systems (DDS) can decrease these effects and can make new therapeutic targets available, certain drugs safer to use, reduce adverse effects and can generally increase the effectiveness of drugs.[3]

To develop a drug delivery system (DDS) based on polymers first a method has to be found to consistently produce and deposit the desired polymer. In addition, it is important to investigate the basic release characteristics of the chosen system. This was the focus of our work thus far.

To achieve a stable and reproducible deposition of polymer (Polypyrrole (PPy), Polyaniline (PANI) and a PPy/PANI system) onto the Pt surface a technique for preparation and synthesis was developed. The preparation protocol focuses on producing an even surface repeatedly and the synthesis protocol focuses on maximizing the amount of deposited polymer while minimizing overoxidation. Ibuprofen (Ibu) was used as placeholder drug. The integration of Ibu into the polymer matrix was achieved by having it present in the reaction solution during the electrochemical polymerization of the monomers. The drug release was monitored and analyzed using UV-Vis-Spectroscopy (see Fig. 1).

We were able to design two DDS based on biocompatible polymers. The first system was made without an additional PANI layer. Electrochemically controlled release of Ibu was achieved with both systems.

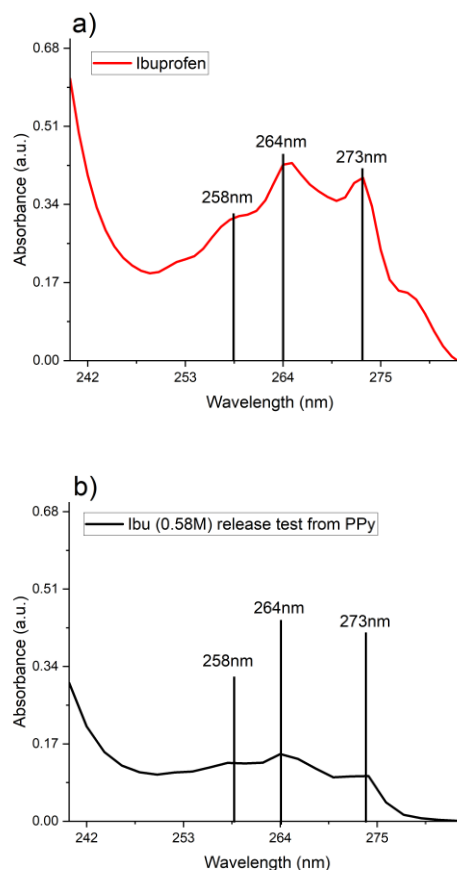


Figure 1. a) Reference spectrum of 0.58M Ibu solution in Acetonitrile with 0.50mM Lithium persulfate. Characteristic peaks are marked. b) Release spectrum of Ibu out of PPy matrix by stimulation with 1.2V.

References

1. Lipinski, C. A. (2000). Drug-like properties and the causes of poor solubility and poor permeability. *Journal of Pharmacological and Toxicological Methods*, 44(1), 235–249.
2. Barrett, J. A., Yang, W., Skolnik, S. M., Belliveau, L. M., & Patros, K. M. (2022). Discovery solubility measurement and assessment of small molecules with drug development in mind. *Drug Discovery Today*, 27(5), 1315–1325.
3. Maranhão RC, Vital CG, Tavoni TM, Graziani SR. (2017) Clinical experience with drug delivery systems as tools to decrease the toxicity of anticancer chemotherapeutic agents. *Expert Opin Drug Deliv.* 2017 Oct;14(10):1217-1226. Epub 2017 Jan 1. PMID: 28042707.

Pea albumin modification by Pulsed Electric Field (PEF)

Raiane Rodrigues da Silva¹, Federico Casanova², and Arunas Stirke¹

¹ Center for Physical Sciences and Technology, Department of Functional Materials and Electronics
Saulėtekio av. 3, LT-10257 Vilnius, email: raiane.rodriques@ftmc.lt

²Food Production Engineering, National Food Institute, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

In response to growing environmental and ethical concerns associated with animal-based food production, such as greenhouse gas emissions, land degradation, and animal welfare issues, consumers are increasingly adopting more sustainable dietary habits (Nascimento et al., 2023). This shift involves reducing the consumption of animal-derived products in favor of plant-based alternatives, with legumes, particularly peas, emerging as a promising protein source (Akharume et al., 2021). Pea protein is primarily composed of globulins (legumin 11S and vicilin 7S) and albumins (2S), each exhibiting distinct structural and techno-functional properties that influence their behavior in complex food formulations (Grossmann, 2024). Although many studies have focused on pea protein as a whole, investigating each fraction individually is crucial to better understand its specific functionalities and potential applications. In particular, a deeper understanding of each fraction may help address challenges commonly associated with pea protein, such as limited solubility and restricted functional versatility compared to animal proteins. To improve their applicability in food systems, non-thermal technologies such as pulsed electric fields (PEF) have emerged as innovative tools for modulating protein structure (Taha et al., 2022).

Thus, this study aimed to evaluate the effect of PEF on pea albumin structure and to compare the influence of different PEF parameters. Pea albumin was hydrated in distilled water overnight. After hydration, the pea albumin solution (10 mg/mL) was subjected to PEF treatment using an electroporator developed by the Center of Physical Science and Technology (Vilnius, Lithuania) (Stankevič et al., 2020). A 0.47 mL aliquot of the suspension was transferred to a Fisher electroporation cuvette (2 mm gap, Thermo Fisher Scientific Inc., Waltham, MA, USA) and exposed to a square-pulse shape with an electric field of 15.6 kV/cm and a pulse width of 5 μ s. Experimental sets were performed by varying (i) the number of pulses (15,

30, and 45) and (ii) the repetition rate (1, 3, and 6 Hz). Electrophoresis, particle size, zeta potential, hydrophobicity, free sulfhydryl groups, and solubility were assessed to evaluate structural modifications.

Regarding the primary structure, electrophoresis analysis revealed no differences in molecular weight, indicating no alterations at this structural level. At the tertiary level, hydrophobicity increased with PEF treatment, with the highest increase observed at 3 Hz and 30 pulses. A similar trend was observed for free sulfhydryl groups. These results indicate that PEF can promote unfolding of the protein, exposing groups that were previously buried in the protein core. Consequently, solubility increased compared to the control. Modifications in particle structure were also observed. PEF treatment reduced particle size, particularly at 1 Hz, demonstrating the ability to disrupt aggregates. Some treatments (1 Hz/15 pulses, 1 Hz/30 pulses, and 3 Hz/15 pulses) also increased zeta potential, possibly due to protein unfolding and the enhanced electrostatic repulsion, which contributed to reduced aggregation. Overall, the results presented here suggest that PEF technology can be an effective approach for inducing structural modifications in pea albumin and that, depending on the applied conditions, different structural outcomes may be observed.

References

1. Nascimento, L. G. L., da Silva, R. R., Odelli, D., Doumert, B., Martins, E., Casanova, F., Marie, R., Carvalho, A. F., Delaplace, G., & de Sá Peixoto Junior, P. P., *Food Res. Int.*, 196, 114982 (2024).
2. Akharume, F. U., Aluko, R. E., & Adedeji, A. A., *Comprehensive Reviews in Food Science and Food Safety*, 20(1), 198–224 (2021).
3. Grossmann, L., *Critical Reviews in Food Science and Nutrition*, 64(23), 8346–8366 (2024).
4. Taha, A., Casanova, F., Šimonis, P., Stankevič, V., Gomaa, M. A., & Stirke, A., *Foods*, 11(11), 1556 (2022).
5. Stankevič, V., Šimonis, P., Zurauskienė, N., Stirke, A., Dervinis, A., Bleizgys, V., Kersulis, S., & Balevicius, S., *Symmetry*, 12(3), 412 (2020).

Synthesis of photoelectrochemically active g-C₃N₄ layers

Kamila Turuta¹, Irena Savickaja¹, Milda Petrulevičienė¹, Jurga Juodkazytė¹

Center for Physical Sciences and Technology, Department of Chemical Engineering and Technology
Saulėtekio av. 3, LT-10257 Vilnius, email: kamila.turuta@ftmc.lt

Photoelectrochemical (PEC) systems are widely investigated as promising platforms for sustainable energy conversion and environmental remediation [1]. Among different semiconductive materials, graphitic carbon nitride (g-C₃N₄) has attracted significant attention due to its metal-free composition, visible-light activity, chemical stability, and low-cost synthesis [2]. The development of efficient g-C₃N₄ layers is essential for improving charge separation, interfacial electron transfer, and overall PEC performance [2].

Compared to traditional metal oxide semiconductors, g-C₃N₄ offers tunable bandgap and high stability under illumination. The intrinsic layered crystal structure of g-C₃N₄ facilitates charge transport and increases the active surface area, enhancing the efficiency of light-driven processes [3]. However, its practical PEC applications are often limited by low conductivity and recombination of photogenerated charge carriers [2], therefore heterostructures with other semiconductors are formed.

In this work, g-C₃N₄ material was synthesized by thermal polymerization of nitrogen-rich precursors, such as melamine or urea, at 550 °C temperature and ambient atmosphere and heterostructures with WO₃ were formed. WO₃ coatings on FTO-coated glass were hydrothermally synthesized at 160 °C using PEG as a structure directing agent [4]. Different g-C₃N₄ layer deposition strategies, such as drop-casting and rolling, were employed to form g-C₃N₄ films on FTO/WO₃ substrates to create heterojunctions. Photoelectrochemical properties of the resulting electrodes were characterized in 0.1 M Na₂SO₄ solution by open circuit potential (OCP), chronoamperometry (CA) and cyclic voltammetry (CV) measurements. Structural and morphological characterization of the coatings was performed using XRD and SEM.

Distinct photoelectrochemical responses were observed for differently modified g-C₃N₄ layers on WO₃ under chopped illumination. The heterojunction prepared by the rolling technique exhibited the highest photoresponse ($\Delta\text{OCP} = 58 \text{ mV}$), nearly twice that of bare WO₃ ($\Delta\text{OCP} = 28 \text{ mV}$) (Fig. 1 (A)). In contrast, the drop-cast heterojunction generated a higher photocurrent (Fig. 1 (B)). A certain enhancement of the photoresponse was observed in heterojunctions, however due to non-uniform surface and poor adhesion of the g-C₃N₄ layer on WO₃-coated FTO substrates, it's challenging to evaluate the actual contribution of g-C₃N₄ to PEC performance. Therefore, further work will focus on alternative deposition strategies, including preparation of heterojunction electrodes by mixing thermally polymerized g-C₃N₄ with non-calcined WO₃ powders, followed by deposition onto FTO and calcination at 400 °C, as well as exploiting the lamellar

structure of g-C₃N₄ to improve charge separation and increase the active surface area through partial exfoliation of stacked layers with concentrated H₂SO₄. Such approaches are expected to provide more uniform coatings, improved photocurrent density, and enhanced long-term performance.

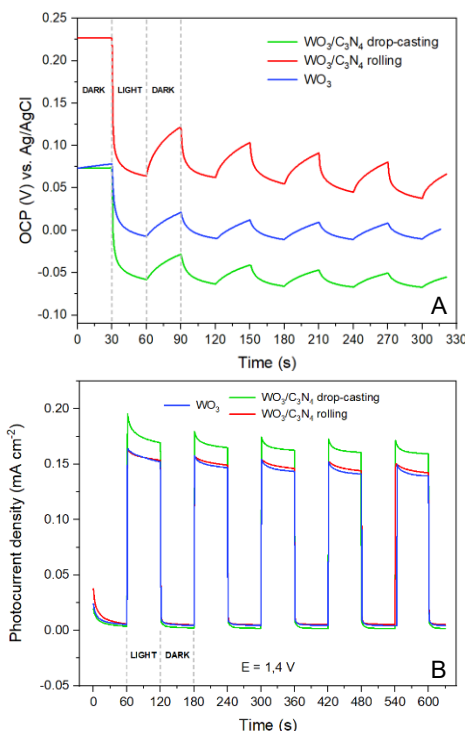


Figure 1. Results of photoelectrochemical measurements with g-C₃N₄/WO₃ and WO₃ electrodes in 0.1 M Na₂SO₄ electrolyte: (A) open circuit potential measured under chopped illumination. (B) Chronoamperometric response measured at E = 1.4 V (vs. Ag/AgCl) under chopped illumination.

References

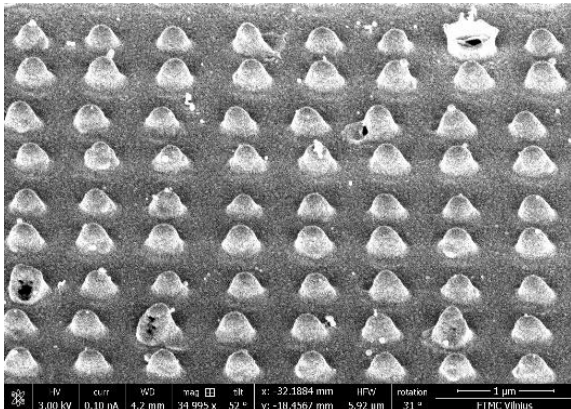
1. R. Liu, Z. Zheng, J. Spurgeon, and X. Yang, "Enhanced photoelectrochemical water-splitting performance of semiconductors by surface passivation layers," 2014. doi: 10.1039/c4ee00450g.
2. H. Zhuang, liqin Lin, M. Xu, W. Xu, and X. Liu, "Construction of g-C₃N₄-based photoelectrodes towards photoelectrochemical water splitting: A review," 2023. doi: 10.1016/j.jallcom.2023.172302.
3. D. Bhandari, P. Lakhani, and C. K. Modi, "Graphitic carbon nitride (g-C₃N₄) as an emerging photocatalyst for sustainable environmental applications: a comprehensive review," 2023. doi: 10.1039/d3su00382e.
4. M. Petruleviciene, K. Turuta, I. Savickaja, J. Juodkazyte, and A. Ramanavicius, "Photoelectrochemical degradation of organic compounds via formed reactive chlorine and sulfate species by WO₃-based photoanodes," *Journal of Electroanalytical Chemistry*, vol. 951, 2023, doi: 10.1016/j.jelechem.2023.117954.

Difrakcinių gardelių periodo ir lazerio impulso energijos tyrimas aukštos kokybės plazmoniniams rezonansams ant ITO padėklų taikant tiesioginį lazerinį rašymą

Marijus Mozdeikis¹, Evaldas Stankevičius¹

¹Fizinių ir technologijos mokslų centras, Lazerinių technologijų skyrius
Savanorių pr. 231, 02300 Vilnius, el. p.: marijus.mozdeikis@ftmc.lt

Plazmoninių nanostruktūrų formavimas ant metalinės dangos yra plačiai nagrinėjamas dėl paviršiaus hidrofobinių savybių, dėl praktinio pritaikymo įvairiuose jutikliuose, medicinoje bei kitose technologijose [1]. Visa tai įmanoma dėl plazmoninio rezonanso, kuris įvyksta šviesai sužadinus ant metalinės dangos paviršiaus esančius elektronus. Žinoma, atsitiktinė krentanti šviesa negali būtų sugerta ir sužadinti elektronų. Šviesos fotonų judesio kiekis yra mažesnis už plazmonų ir jų sąveika nėra galima. Šis neatitikimas kompensuojamas išsklaidant šviesą metalinės dangos paviršiuje tokiu būdu padidinant jos judesio kiekį [2]. Tam tinka metalinės dangos paviršiuje suformuoti nanogumbeliai, kurie veikia kaip difrakcinė gardelė (1 pav.).



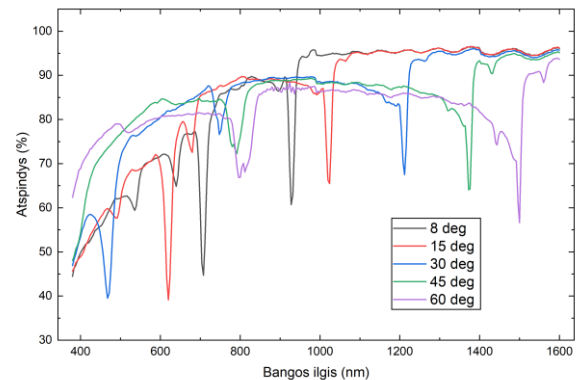
1 pav. Formuojamų sidabro struktūrų nuotrauka daryta su skenuojančiu elektroniniu mikroskopu

Taigi, šio tyrimo metu siekėme suformuoti plazmoninę difrakcinę gardelę naudojant tiesioginį lazerinį rašymą ant ITO stiklo padengto 50 nm storio sidabro sluoksniu. ir atrasti sidabro darinių masyvo formavimo sąlygas (lazerio impulso energiją bei skenavimo greitį), kurias naudojant gardelė pasižymėtų kokybiškiausiais plazmoniniais rezonansais. Rezonansų charakteristikų analizavimui pasitelkėme P-poliarizuotų bei S-poliarizuotų bangų atspindžio spektrus, kuriuose atspindys tikrinamas matomos šviesos – infraraudonųjų spindulių dažnio bangų intervale (2 pav.). Pačių rezonansų kokybę lyginome pagal MQ faktoriaus formulę (1), kurioje įvertinamas jų gylis – h , plotis ties puse maksimalaus gylio – $\Delta\lambda$, rezonansą sukeliančios bangos ilgis – λ_{res} .

$$MQ = \frac{\lambda_{res} \times h}{\Delta\lambda \times 100\%} \quad (1)$$

Atlikome tyrimą 2,8 – 8,4 mm/s skenavimo greičio bei 0,4 – 0,8 nJ lazerio impulso energijos intervaluose, išsiaiškinome, kad geriausios plazmoninių rezonansų charakteristikos ant ITO stiklo padengto 50 nm sidabro sluoksniu pasireiškia formuojant difrakcinę gardelę su

0,5 nJ impulso energija ir 5,6 mm/s skenavimo greičiu. Tokios gardelės plazmoninių rezonansų šviesos



2 pav. Difrakcinės gardelės atspindžio spektras, kuriame matomi plazmoniniai rezonansai, šviesai krentant skirtingiems kampams.

sugerties padidėjimas viršijo 40%, o MQ faktoriaus vertė siekė net 48,42.

Literatūra

- [1] Liudvinavičius R., Vilkevičius K., Stankevičius E., *Applied Surface Science*, 2025, 711, 164127.
- [2] Vilkevičius K., Selskis A., Stankevičius E., *Applied Surface Science*, 2023, 617, 156629.

TERAHERTZ SPECTROSCOPY OF SEMICONDUCTOR METASURFACES IN GaAs BASED STRUCTURES

Barbora Škėlaitė^{1,2}, Vytautas Jakštas³, Aivaras Špokas^{1,2}, Kęstutis Ikamas⁴, Renata Butkutė¹ and Ignas Grigelionis¹

¹Center for Physical Sciences and Technology, Department of Optoelectronics

²Vilnius University, Institute of Photonics and Nanotechnology

³Center for Physical Sciences and Technology, Department of Physical Technologies

⁴Center for Physical Sciences and Technology, Department of Applied Electrodynamics and Telecommunications
Saulėtekio av. 3, LT-10257 Vilnius, email: barbora.skelaite@ftmc.lt

Terahertz (THz) frequency range of the electromagnetic (EM) wave spectrum is known for its unique properties, such as the ability to pass through dielectric materials that are non-transparent to visible light (paper, plastics, wood, textile), that have various applications [1, 2]. Ever-growing field of THz technology, specifically imaging applications, require polarization sensitive, efficient, compact, and easy to operate solid state thermal emitters [3]. Currently, widely known devices, such as quantum cascade lasers or 2DEG plasmonic emitters are cost ineffective, either suffer from limited operating frequency range or require cryogenic temperatures, and contain intricate inner structure that results in complex manufacturing processes [3, 4]. As an alternative, thermal sources providing thermal radiation specifically tailored to narrow emission lines of desired frequency could be used, allowing for the mitigation of the above-mentioned limitations. Such emitters have a structure of a conductive bottom layer, insulating layer and conductive metasurface layer on top, all of which allows for the excitation of magnetic polaritons (localization of magnetic field) as seen in Figure 1.

In this work, the *n*-GaAs/GaAs-based semiconductor emitter structures with intentionally designed *n*-type GaAs metasurfaces for resonant spectral feature excitation in THz frequency range were investigated.

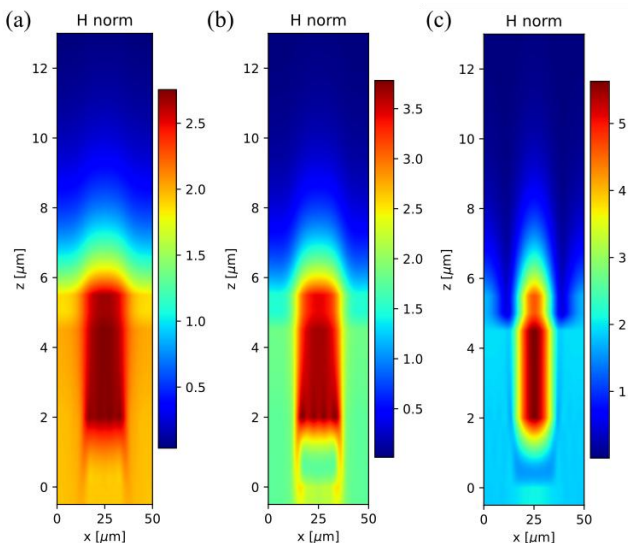


Figure 1. Simulated magnetic field distribution for *n*-GaAs/GaAs structures equipped with semiconductor metasurfaces with different electron concentrations of the *n*-GaAs layers. Simulations were done for electron concentration of $0.5 \times 10^{18} \text{ cm}^{-3}$ (a), $1 \times 10^{18} \text{ cm}^{-3}$ (b)

and $2.1 \times 10^{18} \text{ cm}^{-3}$.

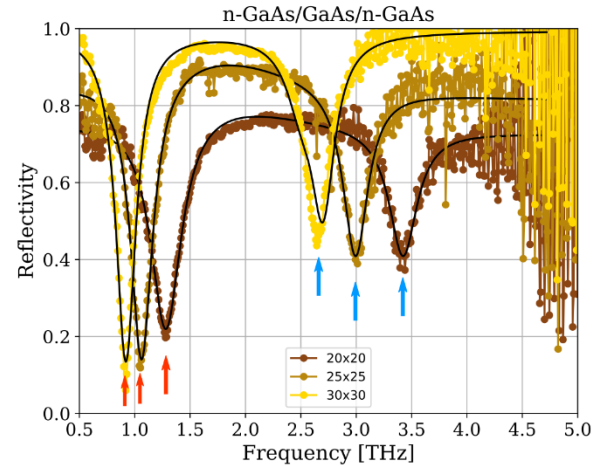


Figure 2. Experimentally measured reflection spectra of *n*-GaAs/GaAs/*n*-GaAs structures with side-length of a square metacell varying from 20 μm to 30 μm. Arrows indicate 1st (red) and 3rd (blue) harmonic resonances.

There were several types of samples fabricated, each comprising either different number of layers, electron concentrations or geometrical parameters of the metasurfaces. Reflectance of sample structures were investigated both theoretically (using Rigorous Coupled Wave Analysis method) and experimentally using THz time-domain spectroscopy. It was observed that resonant frequency of excited magnetic polaritons is dependent on the geometry of the metacell, and material properties. It was determined that the increase in side-length of the metacell leads to the decrease of the resonance frequency (Figure 2). Additionally, due to rectangular-shaped metasurface structure the dual frequency peak can be seen depending on the polarization. Moreover, it was observed that by changing the electron concentration of the *n*-GaAs layers the resonant frequency can be tuned.

References

1. M. Bauer et al., 'Antenna-coupled field-effect transistors for multi-spectral terahertz imaging up to 4.25 THz', Opt. Express, vol. 22, no. 16, pp. 19235–19241, Aug. 2014
2. J. Li et al., 'Rapid sensing of hidden objects and defects using a single-pixel diffractive terahertz sensor', Nature communications, vol. 14, no. 1, p. 6791, 2023.
3. Leitenstorfer A. et al. The 2023 terahertz science and technology roadmap. J. Phys. D: Appl. Phys. 56, 223001 (2023).
4. Bosco L. et al. Thermoelectrically cooled THz quantum cascade laser operating up to 210 K. Applied Physics Letters 115, 010601 (2019).

Methanol Spectroscopy at 257 GHz Employing CMOS-Based Optopair

P. Ivanauskaitė¹, D. Čibiraitė-Lukenskienė¹, N. Rothbart³, H.-W. Hübers^{3,4}, A. Lisauskas^{1,2}

¹Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius. Email: patricija.ivanauskaite@ftmc.lt

²Institute of Applied Electrodynamics and Telecommunications (IAET), Vilnius University, 10257 Lithuania

³Institute of Optical Sensor System, German Aerospace Center (DLR), 12489 Germany

⁴Department of Physics, Humboldt-Universität zu Berlin, 12489 Germany

Terahertz (THz) molecular spectroscopy is a powerful tool for probing molecular and rotational modes [1] of gas molecules, with interest in security, medical diagnostics, climate research, and aerospace.

Although high-end scientific instruments for gas spectroscopy with their methodology exist, a need remains for cost-effective, compact, room temperature solutions. This study explores developing such systems using complementary-metal-oxide-semiconductor (CMOS) technology to reduce component costs, enable large-scale production, and allow real-time room temperature gas spectroscopy.

Study adapted electronic optopair [2] for gas spectroscopy, operating at 255 – 260 GHz frequency range. Experimental setup used a circular THz multipass cell with effective length of 1.9 m [3] and methanol gas was used at various pressures from 0.1 mbar to 1 mbar (setup displayed in Figure 1).

Using a 501 Hz saw-tooth modulation to voltage-controlled harmonic oscillator operating in 255 – 260 GHz range (2000 points/sweep), the system achieved a frequency tuning step size of 2.5 MHz and a total acquisition time of 2 seconds per spectrum (frequency point per 1 ms).

The measured spectra showed a strong correspondence with absorption lines for methanol from the JPL database [3]. The deepest absorption line was at 255.2 GHz and 1 mbar pressure and reaching 13% absorption over 1.9 m long optical path. The observed mismatch at 255.2 GHz absorption line from theoretical values was because of nonlinear frequency vs gate dependency of the emitter. This mismatch can be easily adjusted. The overall accuracy of the spectra was less than 1%, and the signal-to-noise ratio at 1300 Hz modulation was 600:1 when drain voltage for CMOS oscillator was set to 1.3 V.

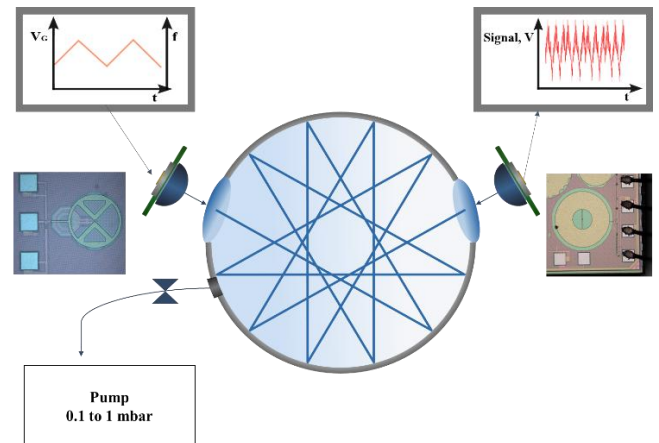


Figure 1. Experimental setup employing CMOS-based emitter and detector pair, and a circular multipass cell with an effective path length of 1.9 m.

This work successfully demonstrated the use of a CMOS-based electronic emitter-detector pair for gas spectroscopy. Initial results show a promising measurement accuracy of better than 1 % in a 2-second sweep time. Future development will focus on integrating emitter, extending frequency tunability, and improving signal-to-noise ratio.

References

1. N. Rothbart, A. Glück, and H.-W. Hübers, "Terahertz Gas Spectroscopy Applied to Medicine and Metrology," *IEEE Transactions on Terahertz Science and Technology*, vol. 14, no. 5, pp. 613–620, Sep. 2024.
2. K. Ikamas, D.B. Butt, A. Cesiul, C. Kolacinski, T. Lisauskas, W. Knap and A. Lisauskas, "All-Electronic Emitter-Detector Pairs for 250 GHz in Silicon," *Sensors*, vol. 21(1), pp. 5795, 2021.
3. Jet Propulsion Laboratory, "Catalog Directory," Apr. 5, 2025. [Online]. Available: <https://spec.jpl.nasa.gov/ftp/pub/catalog/catdir.html>

KVANTINIO DIMERO MODELIAVIMAS SUKABINTAIS KLASIKINIAIS HARMONINIAIS OSCILIATORIAIS

Justina Vaičaitytė¹, Andrius Gelžinis¹, Leonas Valkūnas¹

¹Fizinis ir technologijos mokslų centras, Molekulių darinių fizikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: justina.vaicaityte@ftmc.lt

Nuo pat kvantinės fizikos atsiradimo klasikinės ir kvantinės sistemos buvo lyginamos dėl ryškių jų skirtumų. Klasikinė fizika nagrinėja makroskopinius objektus ir ją remiantis galima bet kuriuo laiko momentu nusakyti jų trajektoriją. Tuo tarpu kvantinė fizika tiria mikroskopines daleles ir gali nusakyti tik tikimybes eksperimento metu stebėti tam tikrą rezultatą. Nepaisant šių skirtumų, kai kurių klasikinių ir kvantinių sistemų matematiniai aprašymai gali būti labai panašūs arba visiškai identiški – tokiu atveju galima laikyti, jog sistemos yra analogiškos.

Akivaizdu, kad daugelyje fizikos sričių kvantinių efektų svarba yra neabejotina. Vis dėlto, tam tikrais atvejais kvantinius efektus galima aprašyti klasikinėmis lygtimis. Daugelio tokių mokslinių darbų tikslas yra parodyti, jog grynai kvantiniais laikyti reiškiniai egzistuoja ir klasikinėse sistemose. Pavyzdžiui, buvo parodyta, jog daugelį iš itin sparčių sužadinimo energijos pernašą fotosintetinėse sistemose lemiančių kvantinių reiškinų galima aprašyti ekvivalenčiomis sukabintų klasikinių osciliatorių lygtimis [1, 2]. Šiame darbe parodoma, jog galima rasti tokią konkrečią klasikinę sukabintų osciliatorių sistemą, kurios laikinė evoliucija visiškai sutampa su kvantinio dimero dinamika.

Šiame darbe nagrinėjama dviejų lygmenų kvantinė sistema, kurią aprašo sužadinimo energijos ε_1 ir ε_2 bei būsenų tarpusavio sąveika J . Remiantis šaltinyje [3] aprašyta metodika ir tankio operatoriaus formalizmu yra gaunamos dvi sukabintos diferencialinės lygtys, aprašančios realios koherentiškumo dalies $q_{12} = \text{Re}(\rho_{12})$ ir užpildų skirtumo $b = \rho_{11} - \rho_{22}$ laikinės evoliucijas:

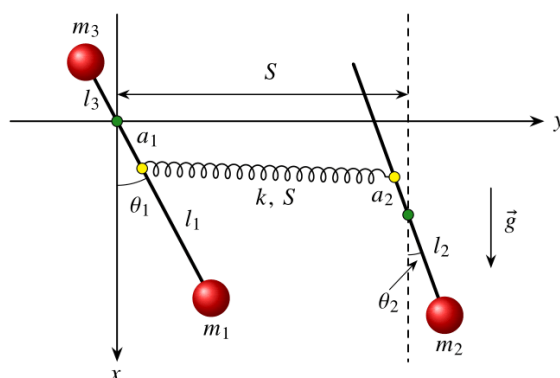
$$\frac{d^2}{dt^2} \begin{pmatrix} q_{12} \\ b \end{pmatrix} = \begin{pmatrix} -\xi^2 & -J\xi \\ -4J\xi & -4J^2 \end{pmatrix} \begin{pmatrix} q_{12} \\ b \end{pmatrix},$$

čia $\xi = \varepsilon_2 - \varepsilon_1$. Parodoma, jog klasikinės sistemos, sudarytos iš trijų karoliukų, pritvirtintų prie strypų galų, kurie tarpusavyje sujungti spyruokle (žr. 1 pav.), matematinis dinamikos aprašymas yra analogiškas kvantinės sistemos dinamikos aprašymui.

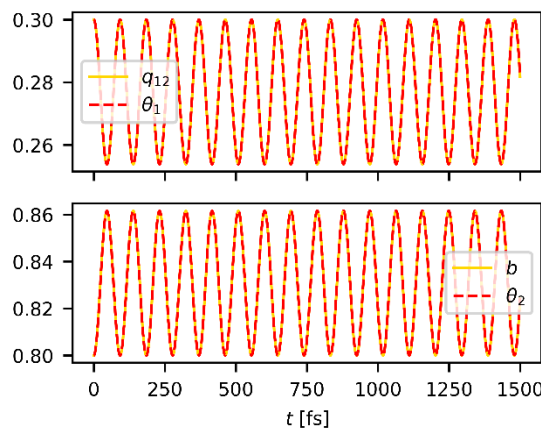
Šioje klasikinėje sistemoje svarbu tai, kad kairiojo strypo pritvirtinimo taškas yra aukščiau spyruoklės prijungimo taško, o antrojo strypo pritvirtinimo taškas yra žemiau spyruoklės prijungimo taško – tokia struktūra lemia neigiamas sistemos sąveikas ir leidžia modeliuoti kvantinę sistemą, kuomet $J > 0$. Kita vertus, parodoma, jog pakėlus spyruoklės kairįjį galą atstumu $2a_1$ (arba nuleidus dešinįjį galą atstumu $2a_2$, žr. pav.), gaunamos lygtys ir atvejui, kai būsenų tarpusavio sąveika yra neigiama. Svarbu paminėti, jog aprašant klasikinę sistemą yra naudojama mažų svyravimų teorija, todėl sistemą aprašančios dinamikos lygtys yra tik apytikslės. Vis dėlto, dėl įvesto pradinių sąlygų ir laiko mastelio kvantinio dimero dinamiką bet kokioms pradinių sąlygų ir laiko vėrtėms. 2 pav. pateikiamas kvantinių ir klasikinių neištiesintų lygčių sprendinių palyginimas esant didelėms pradinių sąlygų

vertėms ($q_{12}^{(0)} = 0,3$, $b^{(0)} = 0,8$). Matosi, kad atitikimas tarp kvantinių ir klasikinių lygčių sprendinių yra puikus.

Jei lygtys, aprašančios kvantinės ir klasikinės sistemų dinamikas sutampa, vadinasi, galima tikėtis, jog abiejose sistemose vyks panašūs reiškiniai. Šio darbo rezultatai turėtų būti naudingi klasikinėms kvantinių sistemų simuliacijoms, taigi tikimės, kad šis darbas stimuliuos tolesnius tyrimus kvantinių-klasikinių analogijų srityje.



1 pav. Trys ant strypų pakabinti karoliukai. Strypų pritvirtinimo taškai pažymėti žaliai, o spyruoklės prikabinimo taškai – geltonai.



2 pav. Kvantinių judėjimo lygčių (geltona linija) ir klasikinių neištiesintų judėjimo lygčių (raudona linija) sprendinių palyginimas. Pradinių sąlygų vėrtės: ($q_{12}^{(0)}, b^{(0)}$) = (0,3, 0,8).

Literatūra

1. T. Mančal, J. Phys. Chem. B **117** (2013).
2. T. Mančal, Chem. Phys. **532**, 110663 (2020).
3. T. E. Skinner, Phys. Rev. A **88** (2013) 012110.

PLOKŠČIŲJŲ THZ OPTIKOS ELEMENTŲ PALYGINIMAS SKAITMENINIAME VAIZDINIMO EKSPERIMENTE

Paulius Kizevičius¹, Sergejus Orlovas¹

¹Fizinių ir technologijos mokslų centras, Optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: paulius.kizevicius@ftmc.lt

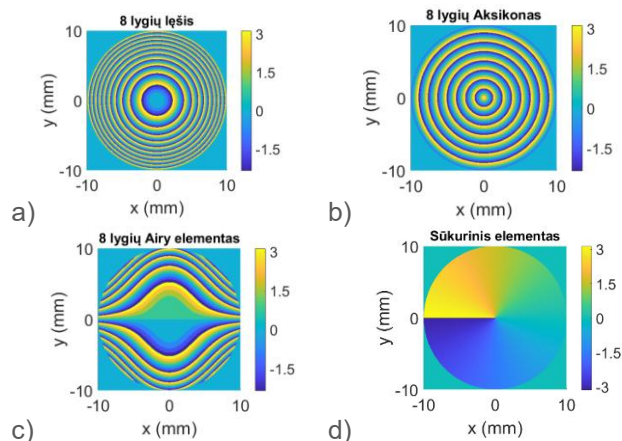
Lazerinėje pramonėje vis didesnę įtaką pluoštų formavimui įgauna fotoniniai plokščiosios optikos elementai. Šie elementai, skirtingai negu tradiciniai sferiniai lęšiai, yra plonesni, lengvesni, kompaktiškesni bei neįneša aberacijų į optinę sistemą. Tokie difrakciniai elementai pagerina objektų vaizdinimo raišką ir leidžia lanksčiai kontroliuoti elektromagnetinių bangų pluošto židinio struktūrą. Būtent pluošto struktūra židinio aplinkoje yra svarbus parametras, dėl kurio netradiciniai lazeriniai pluoštai pritaikomi plačiame elektromagnetinės spinduliuotės dažnių ruože – nuo optinio iki terahercų.

Viena iš svarbesnių specialiosios optikos taikymo sričių yra objektų vaizdinimas, jų atpažinimas, medžiagų detekcija ir bandinių inspekcija. Šios užduotys glaudžiai susijusios su difrakcijos teorija.

Dažniausiai iš lazerio išeinančios spinduliuotės kompleksinį elektrinio lauko skirstinį galime apibūdinti kaip Gauso pluoštą. Sklisdamas šis pluoštas difraguoja nuo pluošto sąsmaukos, o intensyvumas silpnėja. Tai yra viena iš priežasčių, kodėl praktikoje vis didesnę įtaką įgauna taip vadinami nedifraguojantys pluoštai. Vienas tokių yra Beselio pluoštas, kurio skersinio intensyvumo skirstinys nepriklauso nuo atstumo z ir nediverguoja [1]. Kitas yra Airy pluoštas, kuris taip pat išsaugo savo formą, tačiau centrinis maksimumas yra paslinktas ir sklinda išlenkta paraboline trajektorija [2].

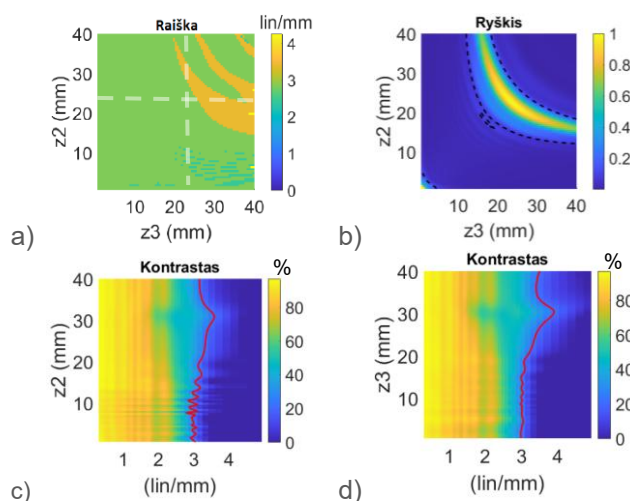
Šie pluoštai paprastai generuojami erdviniais šviesos modulatoriais arba plokščiaisiais fotoniniais difrakciniais elementais, kurie šviesos pluošto frontui priskiria tam tikrą fazinę ir (arba) amplitudinę moduliaciją. Tokios šviesos panaudojimas ir optimalus optinių elementų išdėstymas gali lemti dar aukštesnę vaizdo raišką, ryškumą ir kontrastą, o tai yra vienas pagrindinių vaizdavimo teorijos tikslų [3].

Šiame darbe bus pristatyti sumodeliuoti faziniai difrakciniai elementai ir jų generuojami pluoštai, skirti veikti 0,6 THz ($\lambda = 0,5$ mm) spinduliuotei. Taip pat bus pateikta virtualaus vaizdinimo rezultatų analizė kiekvieno elemento atveju.



pav. 1. Sumodeliuoti faziniai elementai.

Šio darbo idėja – vaizdinimo eksperimente panaudoti ir struktūrinę šviesą. Buvo siekiama išanalizuoti ne tik klasikinio Gauso pluošto THz vaizdinimą, bet ir specialiosios optikos elementų taikymo galimybes. Siekiant palyginti gautų vaizdų kokybę, vertinti raiškos, ryškio ir kontrasto žemėlapiai, taip pat nagrinėta, ar įmanoma pasiekti aukštos kokybės vaizdą didesnėje objekto ir atvaizdo skirtyje, t. y. ar galima pagerinti lauko bei fokusavimo gylį.



pav. 2. Gauso-Gauso vaizdinimo atvejo raiškos a) ir ryškio b) priklausomybė nuo surenkančiojo lęšio (z_2) ir detektoriaus pozicijos (z_3). c) ir d) kontrasto priklausomybė nuo atstumų z_2 ir z_3 ties didžiausio ryškio pozicija. Juoda punktyrinė linija žymi 10% ryškio lygį, raudonas kontūras žymi 20% kontrasto vertės ribą.

Literatūra

1. D. McGloin, K. Dholakia, Bessel beams: diffraction in a new light, Contemporary Physics 46(1), 15–28 (2005).
2. G. A. Siviloglou, D. N. Christodoulides, Accelerating finite energy airy beams, Optics letters 32(8), 979–981 (2007).
3. S. Orlov, R. Ivaškevičiūtė-Povilauskienė, and P. Kizevičius et al., "Light engineering and silicon diffractive optics assisted nonparaxial terahertz imaging," Laser Photonics Rev. 18, 2301197 (2024).

Monte Carlo Study of the Self-assembly of INDO₄ Molecules on Ag Surfaces

Jorūnas Dobilas¹, Evaldas E. Tornau¹

¹Center for Physical Sciences and Technology, Department of Functional Materials and Electronics
Saulėtekio av. 3, LT-10257 Vilnius, email: jorunas.dobilas@ftmc.lt

The spontaneous assembly of organic molecules into ordered structures is the most fascinating phenomena of modern material science, enabling functional nanostructures for applications ranging from nanoelectronics to biomedicine [1].

Surface-confined molecules, governed by subtle intermolecular interactions and substrate effects, can form complex and sometimes unexpected patterns. Among many two-dimensional motifs, the honeycomb structure is the most common molecular pattern that has been realized by molecules of different shapes and sizes. Examples include triangular molecules (TMA, BTB, HTBA) as well as elongated molecules (anthraquinone, TPTC, etc.) on various surfaces, which have been intensively investigated both experimentally and theoretically.

Recently, elongated s-indacene-1,3,5,7(2H,6H)-tetrone molecules (INDO₄) have attracted attention due to their ability to assemble versatile molecular structures on Ag surfaces [2]. A hexagonal framework formed on Ag(111) has demonstrated an unexpected behavior: the central molecule of the hexagon, as evidenced by STM images, switches between two degenerate molecular positions like a molecular rotor. Our aim was to develop a minimal yet predictive model capable of capturing the physics of this ordering.

We constructed a six-state model with four main intermolecular interactions, which was then solved using Monte Carlo techniques. Large scale simulations revealed the complexities of INDO₄ ordering into honeycomb patterns, reproducing and explaining the degeneracy. Using density functional theory, we found that this degeneracy is possible when the hexagonal frameworks are expanded by ~1.4 Å.

A more in-depth analysis and modeling results are presented in Ref. [3].

References

1. A. N. Davis, et al., *Nanoscale* **16**, 21 (2024).
2. N. Kalashnyk, S. Clair *Langmuir* **38**, 3 (2022).
3. J. Dobilas, E. E. Tornau, *Langmuir* **41**, 30 (2025).

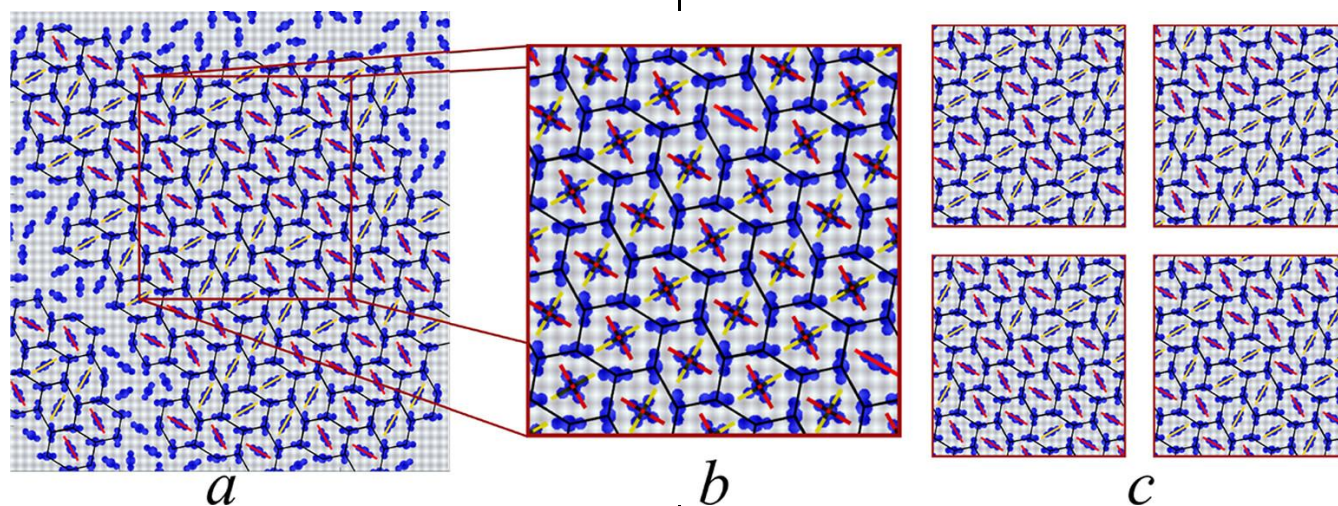


Figure 1. Snapshots of Monte Carlo simulations demonstrating the degeneracy of the hexagonal phases. (a) large-scale pattern, (b) zoomed in section superimposed with (c) degenerate states.

Impact of AlGaAs Barrier Composition and Profile on the Emission of InGaAs Quantum Wells

Justas Žuvelis¹, Andrea Zelioli¹, Monika Jokubauskaitė¹, Aivaras Špokas¹, Bronislovas Čechavičius¹, Evelina Dudutienė¹, Renata Butkutė¹

¹Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius, email: justas.zuvelis@ftmc.lt

Semiconductor emitters operating in the near-infrared (NIR) spectral window have found widespread application in the fields of medicine, optical communications, and the development of sensor technologies. However, the materials employed in these devices still face fundamental limitations. InGaAs/GaAs quantum well (QW) structures, for instance, suffer from temperature stability issues because the GaAs potential barrier is insufficient to effectively confine carriers [1]. This carrier leakage can be mitigated by introducing AlGaAs barriers, but doing so requires careful optimization of barrier composition and profile.

In this study, the optical properties of single InGaAs rectangular QW (RQW) structures containing approximately 21% indium were examined with AlGaAs barriers of varying aluminum content (0%, 12%, 20%, and 30%). The effects of parabolically (PQW) and triangularly (TQW) graded AlGaAs barriers (Fig. 1) on InGaAs QW emission were also explored to evaluate their potential for enhancing carrier confinement. The investigated samples were deposited by molecular-beam-epitaxy, with precise control of growth parameters to minimize interface roughness and defects.

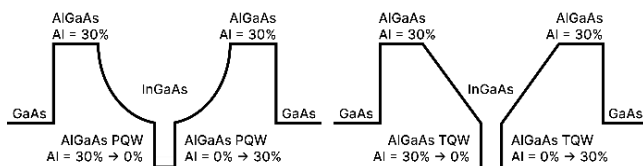


Figure 1. Conduction band schematics of InGaAs quantum wells with (a) parabolically and (b) triangularly graded AlGaAs barriers.

In the case of InGaAs/AlGaAs RQW structures, room-temperature photoluminescence (PL) measurements revealed stronger emission from structures with Al-containing barriers (Fig. 1). This enhancement is attributed to the higher potential barriers, which more effectively suppress carrier thermalization from the QW compared to GaAs. However, at temperatures below 200 K, structures with GaAs barriers showed a stronger PL signal, indicating that Al incorporation results in a higher density of non-radiative recombination centers. Maximizing room-temperature emission therefore requires balancing the competing effects of carrier confinement and crystal quality, with ~12% Al yielding optimal results.

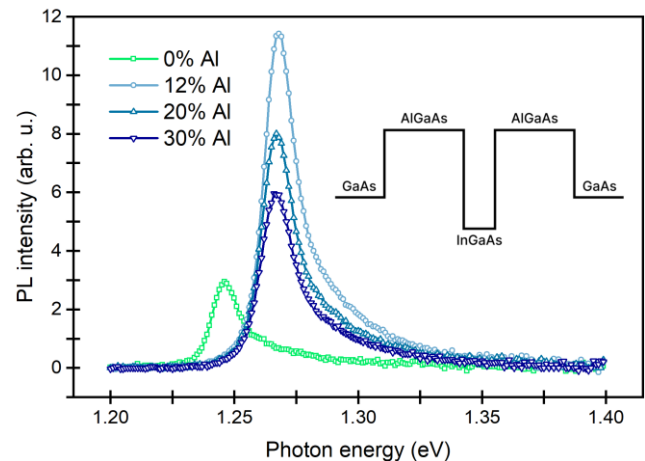


Figure 2. Room temperature PL spectra of the investigated InGaAs/(Al)GaAs RQW structures.

Single InGaAs QW structures with PQW and TQW AlGaAs barriers were found to exhibit stronger PL emission than InGaAs/GaAs RQW structures grown under similar conditions. The higher PL intensity can be attributed to more efficient optical confinement and carrier collection due to the intrinsic electric field [2]. Moreover, the growth conditions required for graded barrier designs, such as increased substrate temperature after QW deposition, were found to induce a blueshift of 10 – 20 meV due to indium segregation.

References

1. H. Dong, J. Sun, S. Ma, J. Liang, T. Lu, Z. Jia, X. Liu, and B. Xu, Phys. Chem. Chem. Phys. 18, 6901–6912 (2016)
2. H. J. Pollard, K. Leo, K. Rother, K. Ploog, J. Feldmann, G. Peter, E. O. Göbel, K. Fujiwara, T. Nakayama, and Y. Ohta, Phys. Rev. B 38, 7635 (1988)

Search for High Triplet Energy Hosts for Stable Blue TADF OLEDs

Giedrius Puidokas¹, Domantas Berenis¹, Gediminas Kreiza¹, Dovydas Banevičius¹, Kristupas Bagdonas¹, Vaida Koženiauskienė², Rita Butkutė² and Karolis Kazlauskas¹

¹ Vilnius University, Faculty of Physics, Institute of Photonics and Nanotechnology, Universiteto st. 3, LT-01513, Vilnius, Lithuania. Email: giedrius.puidokas@ff.vu.lt

² Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilėnų rd. 19, LT-50254, Kaunas, Lithuania.

OLEDs are solid-state devices that use organic materials to emit light and are widely used in displays due to their high contrast, wide viewing angles, and compatibility with flexible substrates. However, the development of efficient, long-lived blue OLEDs remains a critical bottleneck. Degradation in these devices is linked to excitation-induced bond dissociation, emission zone shift and narrowing, and poor charge balance (1). The goal of this work is to investigate various modifications of the benchmark host mCBP and evaluate their performance in blue TADF-OLEDs to identify the derivative that maximizes operational stability. To this end, six host materials were studied (Figure 1): the benchmark mCBP, its tert-butyl and cyano substituted derivatives VJK7 and VJK12, and three derivatives (RB134, RB135, RB134Ph) in which the carbazole units are linked to a biphenyl core through C-C linkages. These materials were designed to host blue TADF emitters by maintaining high triplet energy (≥ 2.8 eV) while improving both charge balance and molecular stability.

The evaluation of the six host materials revealed clear differences in their impact on device performance and stability. VJK7 and VJK12, derived from mCBP by tert-butyl and cyano substitution, introduced steric hindrance that disrupted charge balance without delivering improvements in efficiency or lifetime. RB134 and RB135, with carbazole units linked to a biphenyl core via C-C bonds, altered charge transport behavior and exhibited weakened peripheral C-N bonds (BDE ≈ 0.75 eV), which limited operational stability. RB134 showed bipolar transport and a moderately reduced triplet energy (2.85 eV), while RB135 displayed n-type transport and a significantly lower triplet energy (~ 2.7 eV), making it unsuitable for blue emitters. RB134Ph emerged as the most promising host. Its phenyl-stabilized C-N linkage improved the BDE by ≈ 1.5 eV and maintained bipolar transport. Although its triplet energy (2.82 eV) is slightly lower than that of mCBP, it remains sufficient for use with some blue TADF emitters.

References

1. G. Méhes et al. "Physics and design principles of OLED devices." Handbook of Organic Light-Emitting Diodes 53, p. 1–73 (2020).

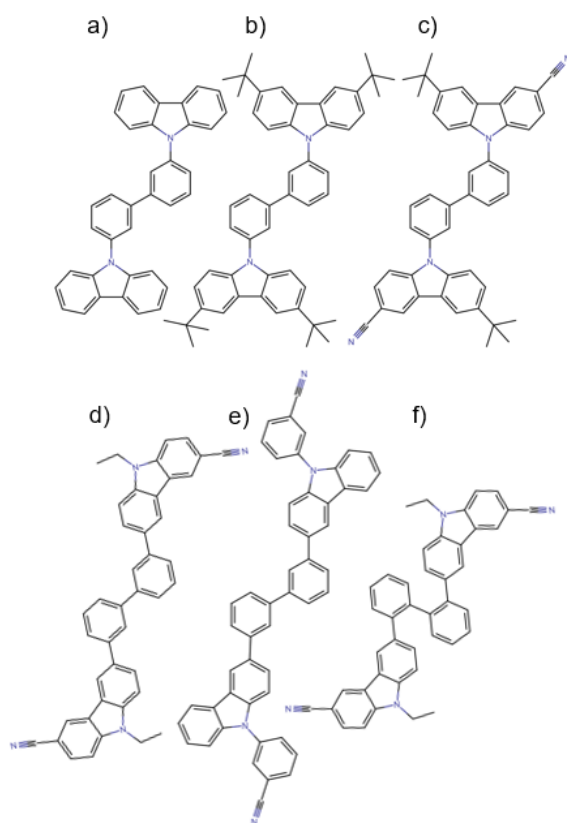


Figure 1. a) mCBP, b) VJK7, c) VJK12, d) RB134, e) RB134Ph and f) RB135 host.

Investigating the effects of urban structure on urban heat island using machine learning

Mehri Davtalab¹, Steigvilė Byčėnienė¹

¹Center for Physical Sciences and Technology, Department of Environmental Research
Saulėtekio av. 3, LT-10257 Vilnius, email: mehri.davtalab@ftmc.lt

The urban heat island (UHI) phenomenon, characterized by elevated temperatures in urban areas compared to their rural surroundings, is primarily driven by anthropogenic activities and modifications of the natural environment. Temperature differences across cities have been extensively recorded and analyzed, with studies consistently attributing them to urbanization and industrialization [1, 2]. Despite its significance as an urban environmental challenge, UHI has only recently attracted focused attention in urban planning research [3]. Effective integration of UHI findings into planning practice requires a detailed understanding of the relationship between land surface temperatures and urban structure.

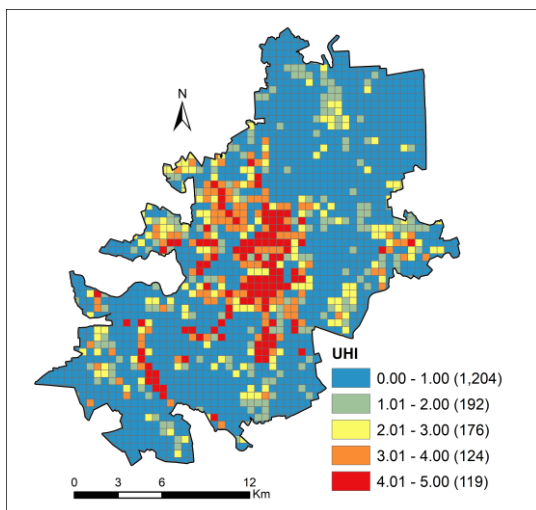


Figure 1: Spatial distribution of UHI in Vilnius, 2022

In this study, UHI data were derived from high-resolution Landsat imagery acquired in 2022 (Fig. 1). We examined both two-dimensional (2D) and three-dimensional (3D) measures of built-up area, together with urban greenery, to assess their influence on UHI intensity. Machine learning (ML) techniques were applied to capture complex and potentially nonlinear relationships between urban structure and UHI, which traditional linear approaches often fail to detect.

The results highlight the critical role of both built-up density and vertical urban structure, as well as the cooling effect of greenery, in shaping spatial clustering of UHI. More specifically, built-up landscape fragmentation intensifies local temperature variability by reducing ventilation and amplifying heat accumulation in densely developed zones.

Acknowledgment

This project has received funding from the Research Council of Lithuania (LMT), agreement No [S-PD-24-137].

References

1. Y. Shen. Separation of the urbanization effects on thermal environment. *Sustainable Cities and Society*, 112, 105585 (2024).
2. Y. Ming, Y. Liu, Y. Li, and Y. Song. Unraveling nonlinear and spatial non-stationary effects of urban form on surface urban heat islands using explainable spatial machine learning. *Computers, Environment and Urban Systems*, 114, 102200 (2024).
3. P. Bansal, P., and S.J. Quan. Examining temporally varying nonlinear effects of urban form on urban heat island using explainable machine learning: A case of Seoul. *Building and environment*, 247, 110957(2024).

IMPROVED EMISSION PROPERTIES OF GaAsBi QWs DUE AlGaAs GRADED BARRIER DESIGN AND THERMAL ANNEALING

Aistė Štaupienė¹, Monika Jokubauskaitė¹, Aivaras Špokas¹, Andrea Zelioli¹, Sandra Stanionytė¹, Bronislovas Čechavičius¹, Renata Butkutė¹, Evelina Dudutienė¹

Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius, email: aiste.staupiene@ftmc.lt

GaAsBi quantum structures are considered a promising material for light sources operating in the near-infrared spectral range, because the incorporation of just a few percent of bismuth into the GaAs lattice significantly redshifts its optical response and reduces the temperature sensitivity of the bandgap energy [1]. Unfortunately, growth of these GaAsBi quantum structures requires very low temperatures, which leads to high defect concentrations and thus lowers the emission efficiency of GaAsBi quantum wells (QWs). Emission intensity can be increased by applying various technological approaches: annealing the structures either *in-situ* in the molecular beam epitaxy (MBE) reactor or *ex-situ* using a rapid thermal annealing (RTA) furnace reduces defect concentrations [2], while the use of non-conventional graded AlGaAs barriers improves carrier capture efficiency [3]. In this work these process strategies were combined, which led to the significant improvement of the optical properties of GaAsBi quantum structures.

We present parabolic GaAsBi/AlGaAs quantum well (PQW) structures that were grown and annealed at different temperatures. It was investigated how the employment of parabolically graded barriers, *in-situ* and *ex-situ* annealing modifies the emission of our samples. The optical properties of these structures were studied by photoluminescence (PL) technique under varying excitation power and as a function of temperature (TDPL).

Room-temperature (RT) spectra of PQW structures showed a PL band of ~1.18 – 1.20 eV, which was attributed to optical transitions in a GaAsBi QW. These structures contained ~3.2% Bi, which was determined by X-ray diffraction. It was observed that RTPL intensity of all GaAsBi graded-barrier structures surpassed the one of a reference sample (a conventional rectangular QW structure), besides the fact that this structure contained three QWs rather than only one. Moreover, the high temperature (HT) growth process (*in-situ* annealing) also resulted in an increase of RTPL peak intensity. Observed PL intensity gain was explained by

the reduction of point defects via HT growth phase, which self-annealed the structures during the MBE growth [4]. Moreover, the intensity of RTPL band also depended on the *ex-situ* annealing temperature. It was found that the optimal RTA temperature correlates with the duration of *in-situ* annealing used during the MBE growth. It was found that *in-situ* annealing can increase the RTPL intensity by ~250%, and an additional optimally chosen *ex-situ* RTA can further double this emission intensity (Fig. 1).

In TDPL measurements structures displayed red-blue-red bandgap shift when temperatures were increased, which showed carrier localization in investigated samples. Samples that underwent *in-situ* annealing exhibited reduced carrier localization, consistent with a more uniform Bi distribution in the GaAsBi layer. Additionally, PL intensity dependence on the temperature was evaluated for PQW structures. Thermal PL quenching decreased for structures grown at HT regime, which was explained by the improved crystal quality via *in-situ* annealing.

All in all, this study revealed that the implementation of PQW design increases PL intensity more than 5 times compared to conventional RQWs. This PL peak intensity can be additionally enhanced ~2.5 times by employing HT-HT growth method. Beyond that, these PQW structures can be *ex-situ* annealed at 700 °C, which results in ~2 times higher PL intensities. Therefore, this study shows that the optimization of structural design, growth and annealing temperatures can boost emission intensities more than 25 times.

This project has received funding from the Research Council of Lithuania (LMTLT), agreement No. S-MIP-24-99.

References

1. R. D. Richards et al., Phys. Stat. Sol. (B), 259, 2100330 (2022).
2. S. Mazzucato et al., Semicond. Sci. Technol., 28, 022001 (2013).
3. S. Pūkienė et al., Nanotechnology, 30, 455001 (2019).
4. J. Mickevičius et al., Phys. Stat. Sol. (A), 210, 1657 (2013).

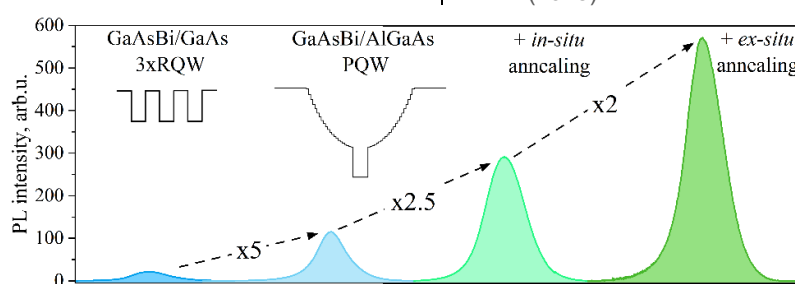


Fig. 1. RTPL spectra of investigated GaAsBi quantum structures.

INTEGRATION OF DIGITAL TERAHERTZ HOLOGRAPHY AND LIGHT SCATTERING MODELING IN GRANULAR MATERIAL ANALYSIS

Lukas Stacevičius^{1,2}, Linas Minkevičius¹, Ignas Grigelionis¹, Agnieszka Siemion³, Rusnė Ivaškevičiūtė-Povilauskienė¹

¹Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio av. 3, LT-10257 Vilnius, email: lukas.stacevicius@ftmc.lt

²Vilnius University, Faculty of Physics
Saulėtekio av. 9, LT-10222 Vilnius

³Warsaw University of Technology, Faculty of Physics
Warsaw, 00-662, Poland

Terahertz (THz) radiation has a unique ability: It can penetrate dielectric materials that are opaque to visible light, which gives opportunity to analyze inner structure of the objects. Additionally, unlike X-rays, THz radiation is non-ionizing, making it safe for human exposure. These properties make THz radiation ideal for various applications, such as security and medicine. THz radiation is widely used for imaging applications to look through or into objects. However, direct imaging does not provide sufficient resolution for small or very thin, layered objects, as only the signal intensity is recorded. This issue can be addressed using coherent imaging methods, one of which is digital THz holography, allowing the recording of both the amplitude and phase information [1].

To analyze the scattering of granular material, a sample consisting of sugar grains with sizes comparable to to terahertz wavelengths was used. Such sample was chosen due to the potential relevance of scattering materials in medical applications. The granules were divided into four size categories: smaller than 125 μm , 125 – 250 μm , 250 – 500 μm , and 500 – 1000 μm . Direct THz imaging and digital THz holography were carried out using a 600 GHz continuous-wave source, with the holographic measurements utilizing two- and four-step phase-shifting techniques [2] (PS2 and PS4, respectively). Direct THz imaging showed a significant decrease in signal intensity with increasing sugar grain size, with lowest intensity observed for the largest grains of 500 – 1000 μm . Compared to direct imaging (see inset of Fig. 1a), digital THz holography distinguished grain sizes more clearly: amplitude reconstructions with PS2 method (see Fig. 1a) showed the clearest contrast between all four size categories, while the strongest contrast of phase reconstruction was achieved with PS4 method (see Fig. 1b). In both PS2 and PS4 reconstructions, the largest grains exhibited the lowest amplitude and the greatest phase difference respectively.

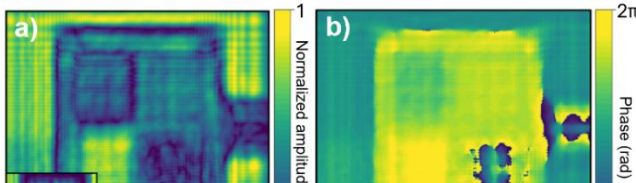


Figure 1. Digital THz holography reconstructions of sugar grains; (a) Amplitude reconstruction using PS2 method; Inset depicts direct THz imaging result; (b) Phase reconstruction with PS4 method.

For Mie scattering modeling, the discrete dipole approximation (DDA) method [3] – well-suited for particles of non-spherical geometry – was used to evaluate light

scattering properties. The largest extinction coefficient was observed for sugar grains in the 500 – 1000 μm range, reaching 38.9 cm^{-1} . The S_{11} and S_{12} elements of the Mueller matrix, describing scattered light intensity over a 180° angular range, were also highest for the largest grains – about 10 000 times greater than for the smallest granules (<125 μm). These results confirmed that granular sizes closest to the THz wavelength of 500 μm produced strongest Mie scattering, as reflected in THz holography by the lowest amplitudes and largest phase differences. Extinction coefficients (see Fig. 2), as well as Mueller matrix elements, were also calculated over the 0.1 – 3 THz frequency range, showing increased light attenuation and scattering intensity with increasing frequency.

In summary, the analysis of sugar grains demonstrated that THz digital holography with phase-shifting techniques can clearly distinguish granular structures of different sizes

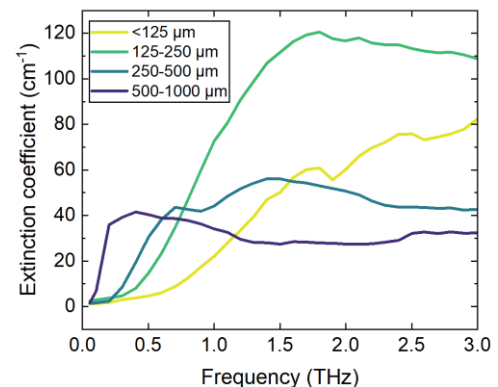


Figure 2. Extinction coefficient dependence on frequency in 0.1 – 3 THz range for sugar grains of four different size categories.

comparable to the radiation wavelength and identify the strongest Mie scatterers, as confirmed by DDA method.

References

1. Sheridan J. T., Kostuk R. K., Journal of Optics, vol. 22, 123002 (2020).
2. Yamaguchi I., Zhang T., Optics Letters, vol. 22, 1268–1270 (1997).
3. Draine B., Flatau P., J. Opt. Soc. Am. A., vol. 11, 1491–1499 (1994).

BEŽYMENIS AmpC BETA-LAKTAMAZĖS APTIKIMAS TAIKANT KOMBINUOTĄ SE/QCM-D METODĄ, PASITELKIANČI SKIRTINGŲ POKLASIŲ IgG ANTIKŪNUS / LABEL-FREE IMMUNOSENSING OF AmpC BETA-LACTAMASE USING COMBINED SE/QCM-D WITH SUBCLASS-DEPENDENT IgG CAPTURE LAYERS

Migle Stanciuskaitė^{1,3*}, Silvija Juciute^{1,3}, Karolina Bielskė², Indre Kucinskaitė-Kodze², Aurelija Zvirbliene², Ieva Plikusienė^{1,3}

¹Faculty of Chemistry and Geosciences, Institute of Chemistry, Vilnius University
Naugarduko g. 24, LT-03225 Vilnius, Lithuania. Email: migle.stanciuskaitė@chgf.stud.vu.lt

²Institute of Biotechnology, Life Sciences Center, Vilnius University
Sauletekio av. 7, LT-10257 Vilnius, Lithuania

³State Research Institute Center for Physical and Technological Sciences
Sauletekio av. 3 Vilnius, Lithuania

Augantis antimikrobinis atsparumas (AMR) verčia ieškoti greitų, be žymenų atliekamų būdų aptikti jį sukeliančius fermentus. Mes išvystėme strategiją AmpC β-laktamazės (rCMY-34) aptikimui, grįstą antikūnais, kartu naudodami spektroskopinę elipsometriją (SE) ir kvarco kristalo mikrogravimetriją su disipacija (QCM-D). Hibridinė sistema leidžia vienu metu įvertinti sausąją (SE) ir hidratuotąją (QCM-D) paviršiaus masę, taip nustatant sluoksnių hidrataciją. Palyginome tris monokloninių antikūnų (mAb) potipius - IgG1, IgG2a ir IgG3 - kryptingai imobilizuotus per baltymą G. Kinetinių ir viskoelastinių duomenų analizė atskleidė mAb potipiams charakteringus skirtumus susidariusiuose sluoksniuose: IgG2a ir IgG3 suformavo labiau prieinamus, vidutiniškai hidratuotus sluoksnius, kurie leido rCMY-34 efektyviau prisijungti (atitinkamai QCM-D dažnio pokytis buvo -50 Hz ir -32 Hz). Sąveikaujant su rCMY-34, mažiausios K_D vertės taip pat gautos IgG2a ir IgG3 atvejais: 2.98×10^{-9} M (IgG2a) ir 1.7×10^{-9} M (IgG3) [1]. IgG1 sudarė kompaktišką sluoksnį, ribojantį fermento prieinamumą (-12 Hz), nors K_D buvo nanomolių eilėje. Prie mAb prisijungusio fermento rCMY-34 sluoksniai buvo labiau hidratuoti ($f_{PBS} = 0.94-0.96$) nei antikūnų monosluoksniai, kurių hidratacija siekė nuo 0.52 iki 0.69. Šie rezultatai pabrėžia, kaip antikūnų potipis ir sluoksnio mechaninės savybės lemia SE/QCM-D biojutiklių veikimą. Ši sistema tiesia kelią nežymėtam β-laktamazių aptikimui, kuris yra kritiškai svarbus AMR stebėsenai. Tolesni darbai bus skirti jautrumo optimizavimui ir suderinamumui su realių mėginių tyrimais.

Rapid, label-free recognition of antibiotic-resistance enzymes is critical for antimicrobial resistance (AMR) surveillance. We developed an antibody-based strategy to detect AmpC β-lactamase (rCMY-34) by integrating spectroscopic ellipsometry (SE) with quartz crystal microbalance with dissipation (QCM-D). The hybrid system enables simultaneous calculation) surface mass density resulting in layer hydration. We compared three monoclonal antibody (mAb) subclasses - IgG1, IgG2a, and IgG3 - immobilized site-directed via protein G. Subclass-dependent differences in the formed capture layers were observed from kinetic and viscoelastic data: IgG2a and IgG3 produced more accessible, moderately hydrated layers that allowed increased enzyme binding with QCM-D response of -50 Hz and -32 Hz, respectively. IgG2a and IgG3 also resulted in lowest K_D values during interaction with rCMY-34, being 2.98×10^{-9} M for IgG2a and 1.7×10^{-9} for IgG3 [1]. IgG1 formed a compact layer with limited analyte accessibility (-12 Hz), despite K_D being in the nanomolar range. Target analyte rCMY-34 monolayers were more hydrated ($f_{PBS} = 0.94-0.96$) than antibody monolayers with hydration ranging from 0.52 to 0.69. Overall, these results highlight how antibody subclass and layer mechanical properties shape the performance of SE/QCM-D immunosensing. This platform provides a pathway towards label-free detection of β-lactamases relevant to AMR monitoring, with further work focusing on sensitivity optimization and real-life sample compatibility.

Literatūra

- [1] K. Bielskė, R. Petraitytė-Burneikienė, A. Avižinienė, J. Dapkūnas, I. Plikusienė, S. Juciutė, M. Stanciuskaitė, A. Žvirblinė, I. Kučinskaitė-Kodze, Broadly reactive monoclonal antibodies against beta-lactamases for immunodetection of bacterial resistance to antibiotics, *Sci Rep* **15** (2025). <https://doi.org/10.1038/S41598-025-04603-2>.

GaAsBi/(Al,Ga)As kvantinių duobių atkaitinimo greito atkaitinimo krosnyje tyrimas

Patricija Strumilaitė^{1,2}, Aivaras Špokas^{1,2}, Andrea Zelioli², Justas Žuvelis^{1,2},

Renata Butkutė², Evelina Dudutienė²

¹Vilniaus universitetas, Fizikos fakultetas
Saulėtekio al. 9, LT-10257 Vilnius, el. p.: patricija.strumilaite@ff.stud.vu.lt

²Fizinių ir technologijos mokslų centras, Optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius

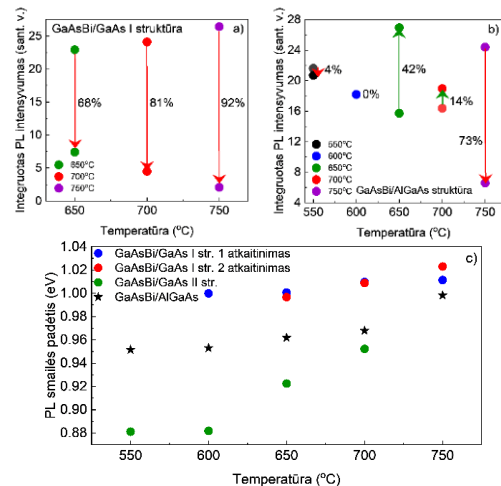
Nedidelį kiekį As atomų GaAs gardelėje pakeitus bismutu, stebimas staigus draustinių energijų tarpo (E_g) mažėjimas (iki 90 meV/1% Bi). Be to, GaAsBi E_g silpniau priklauso nuo temperatūros [1,2]. Dėl šių savybių GaAsBi kvantinės struktūros laikomos perspektyvia medžiaga artimosios infraraudonosios spinduliuotės šaltinių aktyviajai sričiai. Tačiau itin žemos GaAsBi auginimui reikalingos temperatūros (<440 °C [3]) lemia padidėjusią defektų koncentraciją ir mažą fotoluminescencijos (PL) našumą [4]. Vienas iš įprastai taikomų metodų epitaksiškai užaugintų sluoksnių kokybei pagerinti yra jų atkaitinimas aukštesnėje nei auginimo temperatūroje. Vis dėlto šio proceso poveikis GaAsBi struktūroms yra nevienareikšmis [5,6] ir reikalauja tolimesnių tyrimų.

Šiame darbe buvo tiriamos molekulinės pluoštelės epitaksijos (MBE) metodu užaugintos GaAsBi daugybinių kvantinių duobių (MQW) struktūros su GaAs ir AlGaAs barjeriniais sluoksniais. Siekiant ištirti atkaitinimo temperatūros įtaką GaAsBi MQW emisijai, struktūros buvo atkaitintos greito atkaitinimo krosnyje (RTA) 550, 600, 650, 700 ir 750 °C temperatūrose po 3 minutes. Optinės GaAsBi kvantinių struktūrų savybės buvo tiriamos naudojant PL spektroskopiją plačiame 4 – 300 K temperatūrų intervale.

Nustatyta, kad GaAsBi MQW su GaAs barjeriniais sluoksniais atkaitinimas visose tirtose temperatūrose lėmė reikšmingą PL intensyvumo sumažėjimą (žr. 1a pav.). Tai tikėtina susiję su aukštoje temperatūroje vykstančia Bi segregacija, dėl kurios suardoma periodinė GaAsBi/GaAs MQW struktūra.

Tuo tarpu GaAsBi MQW struktūrų su AlGaAs barjeriniais sluoksniais atkaitinimas 650 °C ir 700 °C temperatūrose lėmė atitinkamai 42 % ir 14 % padidėjusį PL intensyvumą (žr. 1b pav.). Tai rodo ne tik pagerėjusią GaAsBi kristalinę kokybę, bet ir tai, kad AlGaAs barjeriniai sluoksniai efektyviai sulaiko Bi atomus kvantinių duobių sluoksniuose. Kitaip nei GaAsBi/GaAs MQW struktūrų atveju, GaAsBi/AlGaAs MQW buvo auginamos pakėlus temperatūrą barjerinių sluoksnių nusodinimo metu, todėl šių struktūrų atkaitinimas iki 600 °C nelėmė jokių pokyčių PL spektruose. Taip pat nustatyta, kad visų tirtų GaAsBi MQW struktūrų atkaitinimas aukštesnėje nei 700 °C temperatūroje pablogina jų optines savybes.

Stebėtas PL juostos mėlynasis poslinkis, užfiksuotas visoms tirtoms GaAsBi MQW atkaitinus aukštesnėje nei



1 pav. Tirtų struktūrų PL intensyvumų palyginimas prieš ir po atkaitinimo a) GaAsBi/GaAs MQW b) GaAsBi/AlGaAs MQW ir c) PL smailės energija visose atkaitintose struktūrose.

600 °C temperatūroje (1c pav.), rodo Bi kiekio GaAsBi sumažėjimą. Šis rezultatas gerai sutampa su literatūroje pateiktas duomenimis [7]. Atkaitinimo metu dalis Bi atomų išeina iš GaAsBi gardelės ir klasterizuojasi, sudarydami Bi kvantinius taškus (QD). Vis dėlto net ir žemoje temperatūroje užregistruotuose GaAsBi/GaAs ir GaAsBi/AlGaAs MQW struktūrų PL spektruose emisija iš Bi QD nebuvo stebima, o spektrų forma prieš ir po atkaitinimo išliko nepakitusi visame tirtame temperatūrų intervale. Tai leidžia daryti prielaidą, kad susiformavusių tinkamo dydžio Bi QD kiekis buvo per mažas, jog būtų galima užregistruoti PL signalą iš Bi QDs.

Finansavimą šiam darbui skyrė Lietuvos mokslo taryba (LMTLT), sutarčių Nr. S-SV-25-203 ir S-MIP-24-99.

Literatūra

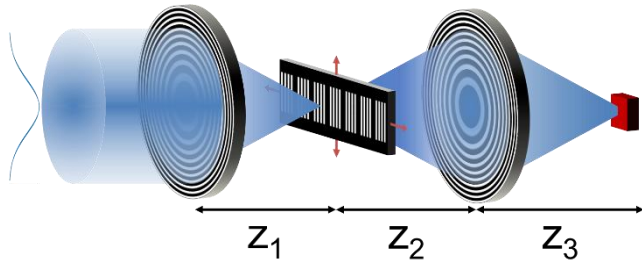
1. S. Francouer, et al., Appl. Phys. Lett., 82(22), 3874-3876 (2003)
2. K. Alberi, et al., Appl. Phys. Lett., 91(5), 051909 (2007)
3. R. Richards, J. Cryst Growth. 390, 120-124 (2014)
4. A. Štaupienė et al Appl. Phys. Lett., 125(22) (2024)
5. P. C. Grant, et al., J. Vac. Sci. Technol. B, 32(2), 02C119 (2014)
6. B. Čechavičius, et al., Semicond. Sci. Technol. 26(8), 085033(2011)
7. R. Butkutė, et al., Nanoscale Res. Lett. 12, 436 (2017)

Fotonių elementų taikymas vieno pikselio THz vaizdinime

Karolis Mundrys¹

¹Fizinių ir technologijos mokslų centras, Optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: karolis.mundrys@ftmc.lt

Šiame darbe pristatomas vieno pikselio terahercų (THz) vaizdinimas, naudojant struktūrinius pluoštus skaitmeniniame eksperimente. Tradicinis vaizdo atkūrimas dažniausiai atliekamas detektorių matricomis, tačiau THz ruože tokios technologijos yra sudėtingos ir nepraktiškos, todėl vieno pikselio vaizdinimo principas tampa itin aktualus. Vietoje dažnai naudojamo erdvinio dažnių filtravimo, šiame darbe buvo taikomas struktūrinės šviesos metodas, apšviečiant bandinį Airy, Beselio, Fibonačio bei Gauso pluoštais. Vaizdinimas buvo atliktas bandinį judinant skersinėje plokštumoje mažais žingsniais. Pagal detektoriaus užregistruojamą signalą bei bandinio poziciją buvo atkuriamas bandinio atvaizdas bei įvertinta jo skyra.

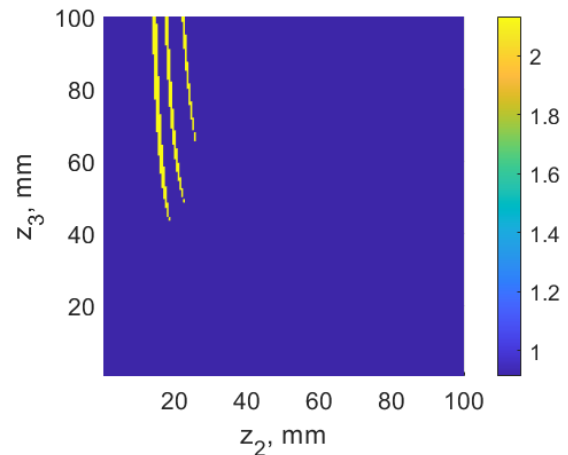


Figūra 1. Vieno pikselio vaizdinimo principinė schema.

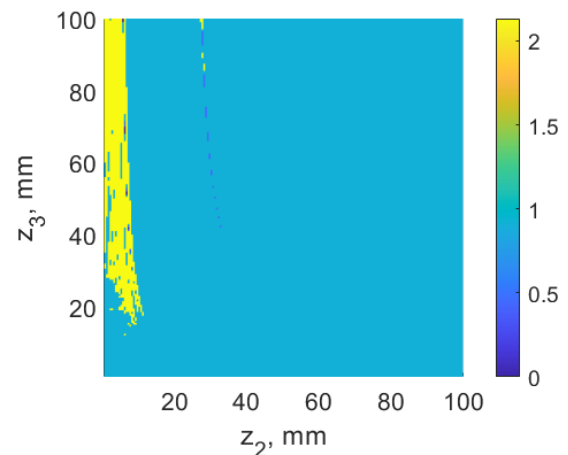
Eksperimento metu buvo nagrinėjama vaizdo kokybės priklausomybė nuo atstumo tarp apšviečiančiojo elemento ir bandinio (z_2) ir atstumo tarp bandinio ir surenkančiojo elemento (z_3). Atstumas tarp apšviečiančiojo elemento ir bandinio (z_1) buvo nustatytas pagal pluošto intensyvumo maksimumą.

Pastebėta, kad vieno pikselio vaizdinimo atveju naudojant klasikinę dviejų zoninių plokštelių konfigūraciją (t.y. sferinių lęšių atitikmuo THz ruože) gaunama gera skyra (~ 2 lin/mm) tik siauruose ruožuose, žr. Figūra 2. Tuo tarpu naudojant Zoninę plokštelę (kaip apšviečiantįjį elementą) bei Airy kaukę (kaip surenkantįjį elementą) gera skyra (~ 2 lin/mm) gaunama plačiame ruože. Skyra ypač nejautri atstumo z_3 pokyčiui, kuris gali svyruoti nuo 30mm iki 100mm praktiškai nekeisdamas vaizdo kokybės.

Gauti rezultatai prisideda prie THz vaizdinimo technologijų plėtros, kuri turi didelį potencialą neinvazinės diagnostikos, storų sluoksnių medžiagų analizės ir kitose srityse. Struktūrinių pluoštų tyrimai leidžia geriau suprasti jų praktinį pritaikomumą ir gali tapti pagrindu efektyvesnių vaizdinimo sistemų kūrimui ateityje.



Figūra 2. Zoninė plokštelės – Zoninė plokštelės konfigūracijos skyros priklausomybė nuo atstumų z_2 ir z_3 .



Figūra 3. Zoninė plokštelės – Airy kaukės konfigūracijos skyros priklausomybė nuo atstumų z_2 ir z_3 .

Literatūra

1. R. Ivaškevičiūtė-Povilauskienė, P. Kizevičius, E. Nacius, D. Jokubauskis, K. Ikamas, A. Lisauskas, N. Alexeeva, I. Matulaitienė, V. Jukna, S. Orlov, L. Minkevičius, G. Valušis, "Terahertz structured light: nonparaxial Airy imaging using silicon diffractive optics" (2022) Light: Science and Applications.

ELECTROCHEMICAL SENSOR FOR SALICYLIC ACID BASED ON A MOLECULARLY IMPRINTED POLYPYRROLE

Gabrielė Slaboševičiūtė^{1,2}, Ernestas Brazys^{1,3}, Vilma Ratautaitė¹

¹ Center for Physical Sciences and Technology, Department of Nanotechnology, Saulėtekio Av. 3, LT-10257 Vilnius. Email: gabriele.slaboseviciute@stud.vilniustech.lt

² Vilnius Tech, Faculty of Fundamental Sciences, Department of Chemistry and Bioengineering, Saulėtekio Av. 11, Vilnius LT-10223, Lithuania

³ Vilnius University (VU), Faculty of Chemistry and Geosciences, Institute of Chemistry, Department of Physical Chemistry, Naugarduko str. 24, Vilnius LT-03225, Lithuania

Salicylic acid, also known chemically as 2-hydroxybenzoic acid, is a precursor and a metabolite of acetylsalicylic acid (aspirin). In addition to its pharmaceutical applications, this compound is often encountered in cosmetics as an ingredient in topical gels, creams, lotions, and solutions. Although permitted for external use, salicylic acid is toxic to humans when ingested and has been classified as an experimental teratogen [1]. Unfortunately, salicylic acid has been reported to be illicitly used as a milk adulterant to prolong shelf life. At low concentrations, the adverse health effects might be mild. However, prolonged exposure can lead to inflammation, vomiting, hyperpnoea, lethargy, cerebral and pulmonary oedema, seizures and even death [2]. Therefore, a quick and easy-to-use system that could help detect and quantify this substance in various food samples is crucial. A molecularly imprinted biosensor could be an excellent tool for detecting salicylic acid in milk samples. In this study, some aspects of molecularly imprinted biosensor development are presented.

Usually, the process of creating a molecularly imprinted polymer involves these steps: i) the self-assembly of pre-polymerisation complexes by combining monomers, crosslinkers, and template molecules in an appropriate solvent; ii) initiation of polymerisation through chemical or electrochemical methods; iii) removal of the template, producing cavities which are specific to the template molecule [3]. This characteristic is advantageous in sensor development.

In this work, the synthesis and characterisation of the molecularly imprinted polymers were performed using electrochemical methods. A screen-printed carbon electrode (SPE) was employed, consisting of a carbon working electrode, a carbon counter electrode, and an Ag/AgCl pseudo-reference electrode. Molecularly imprinted polypyrrole was electropolymerised directly onto the carbon working electrode using chronoamperometry. Following template extraction, the interaction between the polymer and the template molecule was assessed by reintroducing varying concentrations of salicylic acid to the imprinted polypyrrole film on the electrode. The rebinding efficiency was evaluated directly using electrochemical methods, with the analytical signal obtained from the oxidation peak current of salicylic acid in differential pulse voltammetry. The obtained results demonstrate the potential applicability of the developed sensor for salicylic acid analysis.

Acknowledgment: This project has received funding from the Research Council of Lithuania (LMTLT), agreement No. S-LL-25-3.

References

1. Lewis, R. J. *Hazardous Chemicals Desk Reference. Hazardous Chemicals Desk Reference, Sixth Edition* (John Wiley & Sons, Inc., 2008).
2. Choudhary, M. & Sharma, N. Milk Adulterants: Serious Impact on Human Health. *Journal of Medical Evidence* 5, 124–128 (2024).
3. Haupt, K., Linares, A. V., Bompert, M. & Bui, B. T. S. *Molecularly Imprinted Polymers. Topics in Current Chemistry* vol. 325 (Springer, Berlin, Heidelberg, 2011).

RF galios stiprintuvų elgsenos modeliavimas naudojant interpoliuotus atminties polinorus

Andžej Borel¹

¹Vilniaus Gedimino Technikos Universitetas, Kompiuterių ir ryšių technologijų katedra
Plytinės g. 25, 10105 Vilnius, el. p.: andzej.borel@vilniustech.lt

Galios stiprintuvas tai viena pagrindinių šiuolaikinės komunikacinės sistemos fizinės struktūros dalių. Šio komponento parametrai turi lemiamą įtaką sistemos energetiniam bei spektriniam efektyvumui. Stiprintuvų gamyboje naudojami puslaidininkiai pasižymi netiesinę perdavimo charakteristika. Dėl šios priežasties inžinieriai susiduria su dilema – norint suprojektuoti energetiškai efektyvų stiprintuvą tenka jį naudoti netoli puslaidininkio soties būsenos, tai sukuria pastebimus netiesinius perduodamo signalo iškraipymus ir spektro peraugimą už paskirtos dažnių juostos ribų.

Labiausiai paplitęs šios problemos sprendimo būdas yra stiprintuvo perdavimo charakteristikos linearizavimas [1]. Daugiausiai tyrėjų dėmesio sulaukia skaitmeninio išankstinio iškraipymo (angl. *digital predistortion*) linearizavimo metodika. Metodo tikslas – sukurti skaitmeninį filtrą, kuris iškraipytą perduodama signalą taip, kad sudėjus filtro ir paties stiprintuvo iškraipymus rezultate gautume neiškraipytą signalą.

Egzistuoja keli tokio filtro projektavimo būdai. Vienas iš labiausiai paplitusių yra naudojamo stiprintuvo elgsenos modelio (angl. *behavioral model*) apskaičiavimas. Skirtingai nuo modelių, paremtų fiziniiais puslaidininkių procesais, elgsenos modelis išgaunamas iš stiprintuvo įėjimo ir išėjimo signalų palyginimo. Toks modelis reikalauja mažiau skaičiavimų ir yra praktiškesnis realaus laiko sistemose. Pagrindinis tokio modeliavimo būdo trūkumas – modelio rezultatai yra tikslūs tik siaurame stiprintuvo veikimo sąlygų diapazone. Pasikeitus stiprintuvo veikimo sąlygoms pablogėja modelio tikslumas.

Šiame tyrime bandoma išplėsti elgsenos modelio pritaikymą kitiems, negu buvo naudoti modelio apskaičiavime, nešlių dažniams. Paplitę modeliavimo būdai, tokie kaip *atminties polinomas* (angl. *memory polynomials*) yra apskaičiuojami ir taikomi tam tikrame nešlio dažnyje:

$$y_{MP}(n) = \sum_{k=0}^{K-1} \sum_{m=0}^{M-1} a_{km} x(n-m) |x(n-m)|^k, (1)$$

čia $y_{MP}(n)$ – modeliuojamas stiprintuvo išėjimas, $x(n)$ – įėjimas, a_{km} – modelio koeficientai. Modelio koeficientams apskaičiuoti yra išmatuojamas stiprintuvo atsakas tam tikrame nešlio dažnyje. Taikant tiesinės regresijos metodą (1) lygtis išsprendžiama a_{km} atžvilgiu. Bandant pritaikyti gautą modelį nuspėti stiprintuvo atsaką kituose dažniuose, didėja modeliavimo paklaida. 1 paveiksle pateikiama normalizuotos kvadratinės klaidos priklausomybė nuo nešlio dažnio modeliams, apskaičiuotiems prie 3.35 GHz ir 3.55 GHz bandant juos pritaikyti 3.3-3.8 GHz dažnių diapazone. Matyti, kad abiejuose atvejuose modeliavimo paklaida reikšmingai išauga modelį taikant kituose dažniuose.

Norint pagerinti šį rezultatą originalūs atminties

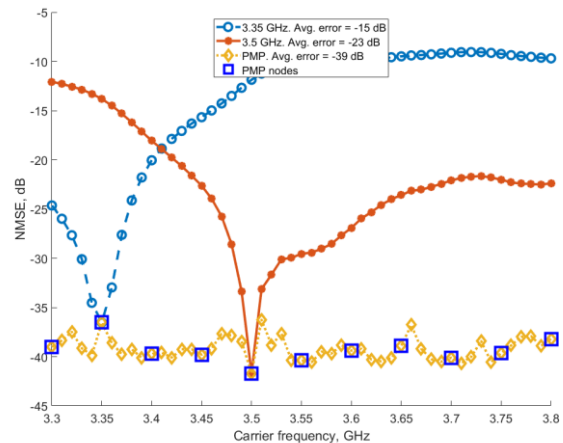
polinomo koeficientai pakeičiami į nešlio dažnio funkcijas $p_{km}(f_c)$:

$$y_{PMP}(n) = \sum_{k=0}^{K-1} \sum_{m=0}^{M-1} p_{km}(f_c) x(n-m) |x(n-m)|^k. (2)$$

Šios funkcijos apskaičiuojamos atlikus N matavimų naudojamame nešlių dažnių diapazone. Surinkti matavimų duomenis naudojami išgauti (1) modelio koeficientus. Visų N modelių koeficientai yra interpoliuojami:

$$\begin{cases} p_{00}(f_c) = F_{int}[(a_{00}; f_{c_0}), (b_{00}; f_{c_1}) \dots (c_{00}; f_{c_N})] \\ p_{01}(f_c) = F_{int}[(a_{01}; f_{c_0}), (b_{01}; f_{c_1}) \dots (c_{01}; f_{c_N})] \\ \vdots \\ p_{km}(f_c) = F_{int}[(a_{km}; f_{c_0}), (b_{km}; f_{c_1}) \dots (c_{km}; f_{c_N})] \end{cases} (3)$$

Tokia modelio struktūra vadinama parametrizuotu atminties polinomu (angl. *parametrized memory polynomial*, PMP).



1 pav. Modeliavimo tikslumo pagerinimas

Pirmame paveiksle pateiktas atminties polinomo, apskaičiuoto iš N = 11 matavimo duomenų rinkinių. Mėlynais kvadratais pažymėti matavimų dažniai. Matyti, kad modeliavimo paklaida reikšmingai sumažėjo. Plačiau apie tyrimą išdėstyta [2].

Literatūra

1. Katz, A.; Wood, J.; Chokola, D. The evolution of PA linearization: From classic feedforward and feedback through analog and digital predistortion. IEEE Microw. Mag. 2016, 17, 32–40.
2. Borel, A.; Barzdėnas, V.; Vasjanov, A. Behavioral Modeling of RF Power Amplifiers with Carrier-Frequency Generalization Using Interpolated Memory Polynomials. Appl. Sci. 2025, 15, 9899.

Nanofilm conductive polymer MIP platform for detection of BSA

Artem Yerniazov¹, Sarunas Zukauskas¹, Alma Rucinskiene², Arunas Ramanavicius^{1,4}

¹Center for Physical Sciences and Technology, Department of Nanotechnology, Saulėtekio av. 3, LT-10257 Vilnius, Lithuania.
Email: artem.yerniazov@chgf.stud.vu.lt

²Center for Physical Sciences and Technology, Department of Electrochemical Material Science, Saulėtekio av. 3, LT-10257 Vilnius, Lithuania.

⁴Department of Physical Chemistry, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University (VU), Naugarduko g. 24, LT-03225 Vilnius, Lithuania.

There is increasing demand for affordable and efficient MIP (Molecularly Imprinted Polymer)-based platforms for biomolecular detection of analytes, such as those in the 50–100 kDa range. A simple yet effective polypyrrole (PPY)-based nanofilm MIP for BSA (Bovine Serum Albumin) is proposed. First, the Pt sheet electrode is pretreated. Then, using a chronoamperometric method, the pre-polymerization solution is electrodeposited onto the surface of the electrode². The template molecule of BSA is passively extracted using a Sodium Dodecyl solution. The sensing mechanism relies on electrochemical impedance spectroscopy (EIS) in phosphate-buffered saline (PBS), where outer-sphere electron transfer occurs between the $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$ redox couple³ and the conductive polymer of PPY². Charge transfer resistance of NIP (Non-Imprinted Polymer) and MIP when BSA is added to the solution are compared. A concentration curve of BSA is created by comparing the R_{ct} (resistance of charge transfer) at each concentration. The LOD and concentration curve demonstrate the sensitivity of the MIP. The imprinting factor is determined by comparing the R_{ct} when equal concentrations of BSA. This approach highlights the feasibility of PPY-based nanofilms for protein imprinting and their potential in low-cost biosensing applications.

References:

1. Leva-Bueno, J., Peyman, S. A., & Millner, P. A., Med. Microbiol. Immunol., 209, 343–362 (2020).
2. Malitesta, C., Mazzotta, E., Picca, R. A., Poma, A., Chianella, I., & Piletsky, S. A., Anal. Bioanal. Chem., 402, 1827–1846 (2012).
3. Lazanas, A. C., & Prodromidis, M. I., ACS Meas. Sci. Au., 3, 162–193 (2023).

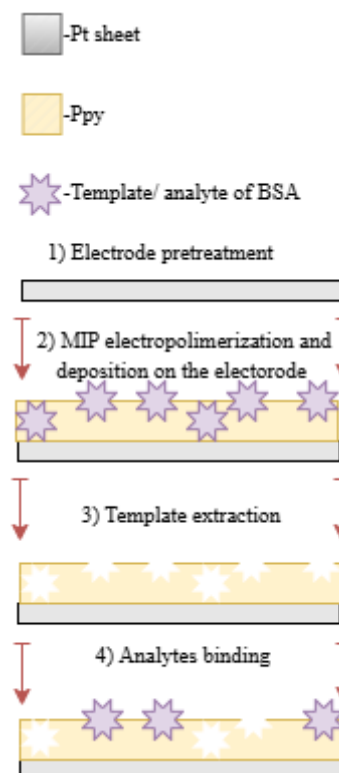


Figure 1. Schematic representation of MIP fabrication with 1) being electrode pretreatment; 2) being the MIP polymerization with the template, 3) is the passive extraction of the template; 4) is the rebinding of the analyte to MIP.

Optimization of Exposure Parameters for SLA-Fabricated SiO₂ Nanoceramic Composites

Danielius Ragoža¹, Nabeel Maqsood¹, Karolis Stravinskas¹, Genrik Mordas¹

¹Center for Physical Sciences and Technology, Department of Laser technologies
Savanorių pr. 231, LT-02300 Vilnius, email: danielius.ragoza@ftmc.lt

Additive manufacturing (AM) has transformed material production by enabling complex, customized designs with high precision and efficiency. Among the various AM techniques, stereolithography (SLA) is particularly notable for its ability to fabricate detailed structures with excellent resolution through layer-by-layer photopolymerization. This study presents the fabrication and optimization of SiO₂-based nanoceramic composites using stereolithography (SLA). A systematic investigation of printing parameters and nanoparticle dispersion techniques was carried out to enhance dimensional fidelity, shrinkage control, and microstructural quality. SLA printing trials employed varying exposure conditions (normal: 5–16 s; bottom: 30–150 s), of which only five parameter sets produced stable specimens. Observation of trial samples demonstrated that short exposures resulted in incomplete curing and poor interlayer bonding, while excessive exposures induced microcracking from photopolymerization stress. Optimal performance was achieved within the 12–16 s normal and 60–90 s bottom exposure ranges, with the G4 parameter set (14 s / 90 s) showing the lowest shrinkage (5.63%), highest ceramic density (1.39 g/cm³), and better dimensional stability. These findings show a process–structure relationship that enhances

the critical role of balanced photopolymerization and effective nanoparticle dispersion in achieving high-quality SiO₂-based nanoceramic composites suitable for advanced applications.

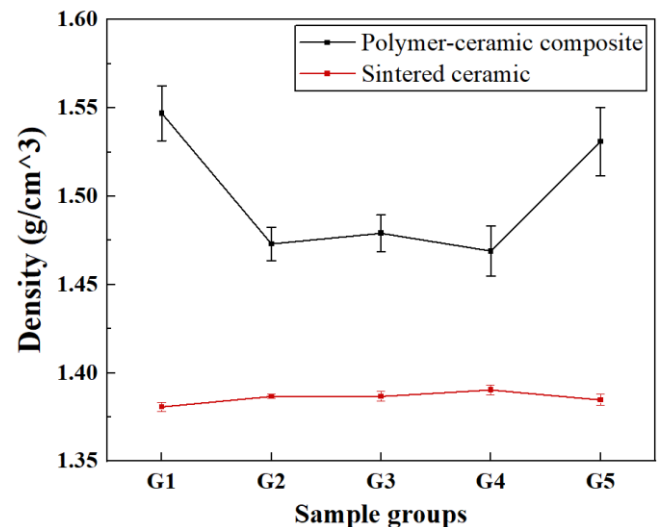


Figure 1. Density comparison between polymer-ceramic composites and sintered ceramic materials for all groups.

Femtosecond laser ablation and polishing of silicon carbide wafers by bibursts

Dainius Ratkus¹, Andrius Žemaitis¹

¹Fizinių ir technologijos mokslų centras, Lazerinių technologijų skyrius
Savanorių pr. 231, 02300 Vilnius, el. p.: dainius.ratkus@ftmc.lt

The electronic industry is evolving every day, aiming to achieve the most efficiently constructed devices. It is essential that these products are developed with a focus on reducing reliance on expensive minerals and minimizing energy consumption, while also being suitable for scalable mass production. Due to its high temperature resistance, hardness, and higher operational lifespan, silicon carbide (SiC) is used in electronic devices that require more durable and long-lasting materials. In the production of SiC wafers chemical mechanical polishing (CMP) is used to reduce the surface roughness. The biggest issue with CMP is that it requires machinery and chemicals needed to obtain an acceptable surface finish of wafers. The production of such wafers with CMP have some negative aspects, such as large amount of material removal, environmental contamination, and low precision. Therefore, the solution of these wafer production problems could be femtosecond laser polishing. Although ultrafast lasers are a relatively expensive tool, they show great potential for SiC wafer processing.

Laser polishing is an alternative technique for reducing surface roughness by inducing molten and re-solidified layers. It is environmentally friendly as it does not require chemicals, pads, or slurries. Therefore, laser polishing could minimize costs and errors when smoothing the surface of such materials. Moreover, laser technology is advancing rapidly in manufacturing and industrial applications, and with this trend, we observe an increased mobilization of laser systems. Therefore, research in materials science and laser parameter optimization must be conducted to ensure that costly minerals are utilized as efficiently as possible.

This study aimed to optimize laser processing parameters to achieve the lowest possible surface roughness and investigate the layer thickness removed per one scan (Figure. 1).

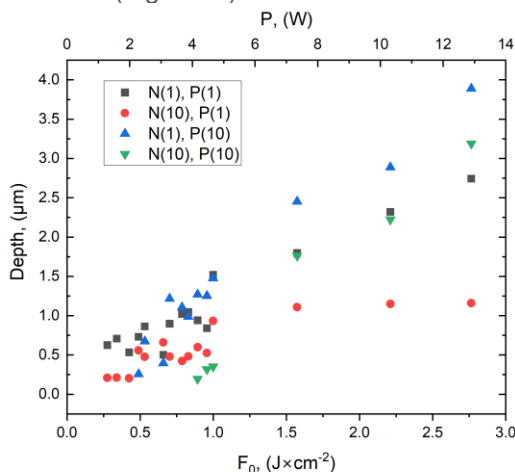


Figure. 1 Ablation depth dependency on laser fluence

and number of pulses in GHz and MHz bursts.

For this task, a femtosecond laser (Carbide, Light conversion) was used for the experiments. The laser had 4 working modes: single-pulse conventional, MHz burst, GHz burst, and burst-in-burst (biburst). Optimization of polishing was performed by varying the number of pulses in GHz and MHz bursts [1, 2]. This optimization technique allowed us to find the optimal laser fluence for the highest ablation efficiency and reach the surface roughness below the initial one (Fig. 2).

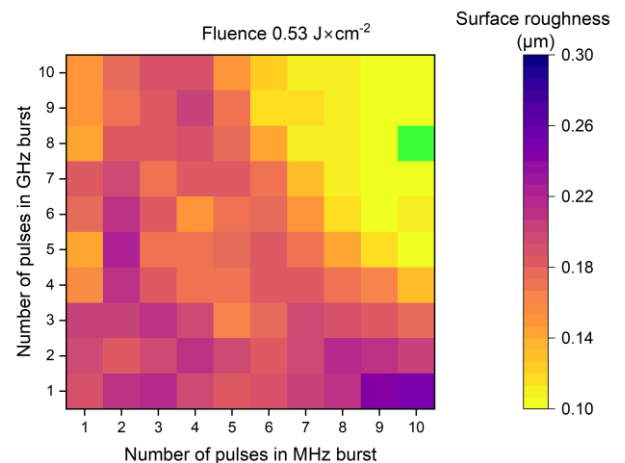


Fig. 2 Surface roughness S_a of laser polished SiC wafer. The number of pulses in MHz and GHz bursts was varied, while the laser fluence was kept at 0.53 J/cm^2 . The green color represents value that is lower than the initial roughness (under 0.1 μm).

Successful laser polishing was performed, reducing surface roughness from 110 nm to 80 nm . The study results demonstrate the potential of laser technology for integration into the SiC wafer production line.

References

1. A. Žemaitis, U. Gudauskytė, S. Steponavičiūtė, P. Gečys, and M. Gedvilas, The ultrafast burst laser ablation of metals: Speed and quality come together, *Opt. Laser Technol.*, **180**, (2025), doi: [10.1016/j.optlastec.2024.111458](https://doi.org/10.1016/j.optlastec.2024.111458).
2. A. Žemaitis, P. Gečys, and M. Gedvilas, Efficient Ablation, further GHz Burst Polishing, and Surface Texturing by Ultrafast Laser, *Adv. Eng. Mater.*, **26**(21), p. 2302262, (2024), doi: <https://doi.org/10.1002/adem.202302262>.

VIENTAZIO PULSUOJANČIO SRAUTO DINAMIKOS IR STRUKTŪROS MIKROKANALUOSE TYRIMAS

Brigita Žakevičiūtė¹

¹Lietuvos energetikos institutas, Šiluminių įrengimų tyrimo ir bandymų laboratorija,
Breslaujos g. 3, LT-44403 Kaunas, el. p.: brigita.zakeviciute@lei.lt

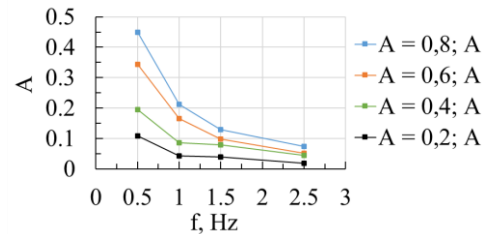
Mikrofluidinės sistemos plačiai taikomos įvairiose mokslo disciplinose, susijusiose su medicina, biologiniais procesais ir inžinerinėmis technologijomis [1-4]. Viena iš aktualių tyrimų kryptių yra nestacionarių srautų analizė, kur svarbu užtikrinti kontroliuojamą proceso efektyvumą, susijusį su medžiagos pernaša, šilumos mainais ir srauto dinamika [5-7]. Pulsuojantis srautas leidžia optimizuoti šių procesų efektyvumą, susijusį su dalelių maišymu, jų atskyrimu, šilumos perdavimu ir energijos nuostolių mažinimu, todėl jo analizė mikrokanaluose reikšminga tiek fundamentiniu, tiek praktiniu požiūriu.

Darbo tikslas – eksperimentiškai ištirti slėgiu sukeltų pulsacijų poveikį vienfazio srauto dinamikai mikrokanaale, taikant skirtingus pulsacijos parametrus ir skirtingos klampos fluidus. Tyrimo metu laikomas nekintantis parametras yra Reinoldso skaičius ($Re = 300$), kintantys parametrai – pulsacijų amplitudė ($A = 0,4; 0,6; 0,8$), dažnis ($f = 0,5; 1; 1,5; 2,5$ Hz), fluído klampa ($\nu = 0,993; 1,613; 3,241$ m²/s⁶). Taip pat analizuojama Womerslio kriterijaus įtaka ($Wo = 0,196–0,866$) greičio profilių pasiskirstymui, lyginant pulsuojantį ir stacionarų tekėjimą. Pabaigoje įvertinama greičio amplitudės priklausomybė nuo pulsacijų dažnio. Tyrimui atlikti naudotas pastovaus skerspjūvio, kvadratinio profilio mikrokanaalas. Tiriamaisiais fluideis pasirinktas vanduo (A) ir du skirtingos koncentracijos ($B – 18\%$ ir $C – 36\%$) vandens ir glicerino mišiniai. Stacionaraus ir pulsuojančio srauto įtekėjimo sąlygos generuojamos naudojant aukšto slėgio rezervuarą ir valdymo bloką, o pulsuojantis srautas sukuriamas varijuojant slėgį kanalo įtekėjime pagal sinuso dėsnį. Matavimai atlikti taikant mikrosrautų vizualizacijos metodą, paremtą indikacinių mikrodalelių poslinkio matavimo principu, kuris apskaičiuojamas taikant kryžminės koreliacijos metodą.

Gauti rezultatai parodė, kad pulsuojančio srauto greičio profiliai praktiškai sutampa su stacionaraus srauto profiliais, sūkurinių struktūrų nepastebėta, hidrodinaminame stabilizacijos ruože nusistovėjęs laminarinis tekėjimas. Wo kriterijaus įtaka tyrime greičio profilių pasiskirstymui buvo minimali, kai $Wo < 1$, nes klampumo jėgos dominuoja prieš momentines inercijos jėgas.

Klumpumo jėgoms kompensuoti buvo didinamas slėgis įtekėjime, kad būtų išlaikyta Re vertė, todėl srauto vidutinis greitis taip pat išaugo. Keičiant pulsacijų amplitudę, vidutinis pulsuojančio srauto greitis nekito – kito tik momentinės greičio vertės.

Pastebėta, kad didėjant dažniui srauto maksimalus greitis mažėjo, todėl nustatant absoliutinio greičio pulsacijos kreivės maksimumo ir minimumo taškus, apskaičiuota tikroji amplitudė, kuri parodė, kad greičio amplitudė turi atvirkščią priklausomybę pulsacijų dažniui. (1 pav.)



1 pav. Greičio amplitudės priklausomybė nuo dažnio: Vanduo (A)

Atliktas tyrimas parodė, kad greičio amplitudės sumažėjimas įvyko ne dėl pasikeitusių slėgio įtekėjimo sąlygų, o dėl pulsuojančio srauto elgsenos atsako į didėjantį dažnį, nes slopinamas greičio atsakas. Didžiausias pokytis nustatytas vandens atveju. Šis efektas atsirado dėl fluído tekėjimo metu patiriamų nuostolių, susijusių su trintimi ar inercija mikrokanaale, kas bus nustatyta tolimesniuose tyrimuose.

Gauti rezultatai papildė fundamentines žinias apie pulsuojančio srauto dinamiką mikrokanaluose ir gali būti pritaikomi projektuojant mikrofluidines sistemas, kuriose būtina valdyti nestacionarius srautus.

Literatūra

1. B. Dincau et al., *Small* 16, e1904032 (2020).
2. X. Wu et al., *Cardiovasc. Eng. Technol.* 13, 428–442 (2022).
3. X. Xu et al., *Biomech. Model. Mechanobiol.* 19, 1679–1695 (2020).
4. A.-I. Garcia-Moreno et al., *Int. J. Adv. Manuf. Technol.* 117, 1825–1841 (2021).
5. M. T. Abdelghany et al., *J. Therm. Anal. Calorim.* 148, 6169–6182 (2023).
6. F. T. MAHMOOD, et al., *Results Eng.* 17, 100941 (2023).
7. C. Li. et al., *Can. J. Chem. Eng.* 100, 2608–2622 (2022).

DESIGN AND APPLICATION OF MXENE-NOBLE METAL NANOSTRUCTURE COMPOSITES FOR COLOURIMETRIC WATER QUALITY TESTING

Gintarė Ruginytė^{1,2}, Agnė Sukovienė², Saqib Ali², Simonas Ramanavičius², Arūnas Ramanavičius¹

¹Center for Physical Sciences and Technology (FTMC), Department of Nanotechnology
Saulėtekio Av. 3, LT-10257 Vilnius. Email: gintare.ruginyte@gmc.stud.vu.lt

²Center for Physical Sciences and Technology (FTMC), Department of Electrochemical Material Science
Saulėtekio Av. 3, LT-10257 Vilnius.

Colourimetric sensors are widely employed in biological and environmental analyses due to their low cost, operational simplicity, and ease of use. These sensors are capable of detecting a variety of organic and inorganic species, including proteins, amino acids, nucleic acids, viruses, and heavy metal ions in real samples. However, they also present limitations, such as low extinction coefficient, limited selectivity, and reduced sensitivity [1].

Advanced two-dimensional (2D) nanomaterials are promising adsorbents for sensing platforms. Incorporation of 2D nanomaterials can enhance sensor sensitivity and selectivity by exploiting their high surface area and tunable physicochemical properties. The integration of these materials enables the development of more versatile and efficient sensors in water quality monitoring [2]. MXenes, a novel class of 2D materials first reported in 2011, have attracted growing attention due to their large specific surface area and physicochemical properties. Among these, $\text{Ti}_3\text{C}_2\text{T}_x$ is one of the most extensively studied water-stable MXenes with hydrophilic properties and electrostatic interactions, suitable for adsorption-based sensing applications [3][4].

This research focuses on the synthesis of titanium carbide MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) and its surface modification with noble metal particles, such as gold (Au) and silver (Ag). A MXene-based sensor was developed for the colourimetric detection of organic molecules in aqueous media. The formation of Au and Ag nanoparticles on the MXene surface was confirmed by UV-Vis spectroscopy, showing characteristic surface plasmon resonance peaks at approximately 580 nm for Au and 440 nm for Ag, with intensity changes correlating with analyte concentration.

The objective of this study is to utilise MXene modified with Au and Ag nanoparticles as an optical probe for the colourimetric detection of L-cysteine in aqueous media, with the aim of enhancing selectivity and sensitivity. L-cysteine was selected as a model analyte due to its thiol group, which interacts strongly with Au and Ag nanoparticles, thereby enabling effective evaluation of the sensor's performance. Moreover, amino acids such as L-cysteine are typically absent in municipal and drinking water. Therefore, their detection may serve as an indicator of contamination from industrial, agricultural, or biomedical sources. The obtained results indicate that the developed MXene-based sensor provides a promising approach for L-cysteine detection.

References

1. Y. Wu, J. Feng, G. Hu, E. Zhang, and H. H. Yu, "Colorimetric Sensors for Chemical and Biological Sensing Applications," *Sensors* 2023, Vol. 23, Page 2749, vol. 23, no. 5, p. 2749.
2. D. Zhu, B. Liu, and G. Wei, "Two-Dimensional Material-Based Colorimetric Biosensors: A Review," *Biosensors* 2021, vol. 11, no. 8, p. 259.
3. I. Navitski, A. Ramanaviciute, S. Ramanavicius, M. Pogorielov, and A. Ramanavicius, "MXene-Based Chemo-Sensors and Other Sensing Devices," *Nanomaterials* 2024, Vol. 14, Page 447, vol. 14, no. 5, p. 447.
4. S. Adomavičiūtė-Grabusovė, S. Ramanavičius, A. Popov, V. Šablinskas, O. Gogotsi, and A. Ramanavičius, "Selective Enhancement of SERS Spectral Bands of Salicylic Acid Adsorbate on 2D $\text{Ti}_3\text{C}_2\text{T}_x$ -Based MXene Film," *Chemosensors* 2021, Vol. 9, Page 223, vol. 9, no. 8, p. 223.

Formation of H, C, Si, La Ion targets to use in the Negative Cs-sputtering Ion source Hiconex

Deividas Rūškys¹, Mindaugas Gaspariūnas¹, Konstantinas Birzul¹, Vitalij Kovalevskij¹

¹Center for Physical Sciences and Technology, Department of Nuclear Research
Savanorių av. 231, LT-02300 Vilnius, email: deividas.ruskys@ff.stud.vu.lt

The performance of negative ion sputtering sources is strongly influenced by the physical and chemical properties of the sputtering target, making the careful preparation and conditioning of suitable ion targets essential for achieving high and stable negative ion yields. In this work, a series of experimental studies were carried out to investigate the formation and optimization of sputtering targets for negative ion production in a Hiconex-type cesium sputtering ion source. The research was aimed at understanding how target composition, surface modification, and operating conditions affect both the short-term efficiency and long-term stability of negative ion emission.

A range of target materials including selected metals, semiconductors, and compound materials with different electron affinities and target shapes were fabricated, mounted in the Hiconex ion source, and tested under controlled sputtering conditions. The prepared targets were exposed to sputtering plasma with varying beam parameters, while their surface state was systematically conditioned through cesium deposition, controlled heating, and exposure to reactive gases in order to tailor work function and electron capture probability.

Overall, the experimental results highlight the critical role of both material selection and surface conditioning in the preparation of suitable ion targets for negative ion sources. The results not only contribute to the operational optimization of Hiconex-type sources but also have broader implications for accelerator-based applications and will be used for the properties of THz detectors and sources modification using high energy ion beams provided by the Tandetron 4110A ion accelerator.

References

1. Middleton, R., (1989), A Negative-Ion Cookbook, University of Pennsylvania, 194 p.



Figure 1. Negative Cs-sputtering Ion source target

Target performance was evaluated in detail using a dedicated Hiconex ion source setup integrated into a Tandem-type Tandetron 4110A accelerator. Negative ion production was characterized through direct current measurements, energy-resolved ion spectra, and target efficiency evaluation. The experiments demonstrated that metallic targets treated with cesium exhibit a pronounced enhancement in negative ion output, primarily due to the significant lowering of the effective surface work function. Comparative studies further revealed that semiconductors and compound materials, although often producing lower absolute ion currents, displayed favorable stability characteristics, making them attractive for long-duration applications.

PLASMON-EXCITON POLARITONIC EMISSION LIFETIME DYNAMICS UNDER STRONG COUPLING

Evita Spalinskaitė¹, Povilas Jurkšaitis¹, Justina Anulytė¹, Ernesta Bužavaitė -Vertelienė¹, Vytautas Žičkus^{1,2}, Dovydas Banevičius³, Karolis Kazlauskas³ ir Zigmas Balevičius¹

¹ Center for Physical Sciences and Technology, Department of Laser Technologies, Plasmonics and Nanophotonics Lab., Saulėtekio av. 3, LT-10257 Vilnius, email: evita.spalinskaite@ftmc.lt

² School of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, UK

³ Vilnius University, Faculty of Physics, Institute of Photonics and Nanotechnology, Saulėtekio av. 3, LT-10257 Vilnius, Lithuania

Plasmonics play an important role in the development of coherent light quantum nano-emitters for advanced optical sensing and integration with electronic circuits. Surface plasmons are coherent oscillations for free electrons and under appropriate conditions can directly interact with light to form surface bound states known as surface plasmon polaritons (SPPs). SPPs when coupled with emitters in the near field, are widely used to enhance various optical processes such as fluorescence [1], lasing [2], Raman scattering [3]. In the strong coupling regime, spontaneous emission rates can be enhanced or suppressed, which affects the fluorescence lifetime of emitters. A deeper understanding of coherent energy exchange dynamics can be valuable for advancing quantum optical sensing. In this project we explored the polariton dynamics of the strongly coupled Rhodamine 6G (R6G) and SPPs using total internal reflection ellipsometry (TIRE), photoluminescence spectroscopy and total internal reflection fluorescence (TIRF) microscopy [4].

The main sample consists of a thin metal (Ag) film with PMMA-R6G layer deposited on a glass substrate (CS). With TIRE method the plasmon-exciton dispersion relation was extracted, which revealed clear bending compared to single SPP and single PMMA-R6G cases, confirming strong coupling between the SPP and R6G dye exciton. Angle dependent photoluminescence measurements showed modified emission spectrum under non-resonant excitation conditions. One of the peaks displayed angular dependence and behavior similar to lower polariton branch, while another represented uncoupled dye molecules. Finally, fluorescence lifetime extracted from TIRF microscopy measurements decreased when the laser incident angle exceeded 18.4°. In this study we present the concept for the fluorescence decay mechanism from polaritonic state interacting with exciton reservoir, where we define exciton reservoir as uncoupled molecules remaining after initial excitation of polaritonic state. The interplay between different polariton dynamics mechanisms is observed by gradually transitioning from non-resonant excitation conditions primarily linked with bare exciton, to resonantly pumping upper polariton state.

In summary, various experimental techniques were implemented to investigate plasmon-exciton emission dynamics. The results demonstrate strong coupling, angle dependent spectral shifts and excitation dependent fluorescence lifetimes. By varying the detuning parameters of strong coupling regime with

experimental scheme, we can effectively enhance or suppress coupling due to increased resonant excitation conditions. In our case the measured lifetimes cannot be explained without the influence of additional energy level in emission dynamics, such as incoherent transition from exciton reservoir to lower polaritonic branch. The fundamental understanding of coherent energy exchange dynamics has potential importance for development quantum optical nanodevices, polariton lasers, polariton condensation.

References

1. Kühn, S., Håkanson, U., Rogobete, L., & Sandoghdar, V., *Phys. Rev. Lett.*, 97(1), 017402 (2006).
2. Seidel, J., Grafström, S., & Eng, L., *Phys. Rev. Lett.*, 94(17), 177401 (2005).
3. Wei, H., & Xu, H., *Nanoscale*, 5(22), 10794 (2013).
4. Jurkšaitis, P., Anulytė, J., Spalinskaitė, E., Bužavaitė-Vertelienė, E., Žičkus, V., Banevičius, D., Kazlauskas, K., & Balevičius, Z., *Nanophotonics*, 14(14), 2485–2493 (2025).

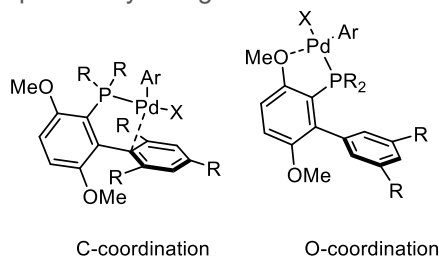
Electron-deficient phosphine ligands for palladium catalysed C-N cross-coupling reactions

Jonas Paukštys^{1,2}, Tomas Paškevičius¹, Linas Labanauskas¹

¹Center for Physical Sciences and Technology, Department of Organic Chemistry,
Akademijos st. 7 LT-08412 Vilnius

²Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko st. 24, LT-03225 Vilnius
jonas.paukstys@ftmc.lt

Arylamines are widely encountered as parts of pharmaceuticals¹, ligands², herbicides and fungicides³. Palladium catalysed C-N cross-coupling reactions are frequently applied in the synthesis of these compounds. Despite extensive research in this area, coupling of heteroaryl compounds remains a challenging task. In 2024 novel O-bound electron deficient phosphine ligands (Figure 1.) were shown to be resistant to deactivation processes encountered in reactions with heteroaryl compounds.⁴ Modification of steric and electronic properties of these could enable reactions previously thought to be unfeasible.



C-coordination O-coordination
Figure 1. C- and O- coordinated ligands

In this work various electron-deficient ligands were synthesized from biaryl backbones and dialkyl phosphines. (Figure 2.).

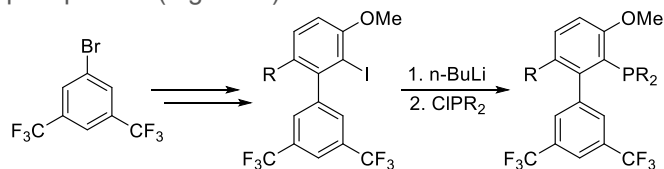


Figure 2. Synthesis of ligands

After the optimisation of reaction conditions ligands were tested with various heteroaromatic substrates.

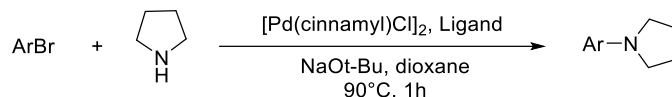


Figure 3. C-N cross-coupling

Substrates such as 2-bromo pyridine, 3-bromo pyridine, 5-bromo pyrimidine were successfully used in this reaction.

References

1. Roughley, S. D.; Jordan, A. M. The Medicinal Chemist's Toolbox: An Analysis of Reactions Used in the Pursuit of Drug Candidates. *J. Med. Chem.* 2011, 54, 3451–3479.
2. Ruiz-Castillo, P.; Buchwald, S. L. Applications of Palladium-Catalyzed C–N Cross- Coupling Reactions. *Chem. Rev.* 2016, 116, 12564– 12649.
3. Devendar, P.; Qu, R.-Y.; Kang, W.-M.; He, B.; Yang, G.-F. Palladium-Catalyzed Cross-Coupling Reactions: A Powerful Tool for the Synthesis of Agrochemicals. *J. Agric. Food Chem.* 2018, 66, 8914– 8934.
4. Feng, K.; Elaine Reichert Raguram; Howard, J. R.; Peters, E.; Liu, C.; Sigman, M. S.; Buchwald, S. L. Development of a Deactivation-Resistant Dialkylbiarylphosphine Ligand for Pd-Catalyzed Arylation of Secondary Amines *J. Am. Chem. Soc.* 2024 146 (39), 26609– 26615.

Comprehensive Literature Review of Thermal and Electrical Challenges in Electro-Optic Pulse Drivers

Edgard Aleinikov¹, Vaidotas Barzdėnas¹

¹Department of Computer Science and Communications Technologies, Vilnius Gediminas Technical University, 10105 Vilnius, Lithuania; edgard.aleinikov@vilniustech.lt

Pockels cells are electro-optic devices used in advanced laser systems, they require precisely controlled, nanosecond-scale high-voltage pulses with amplitudes of several kilovolts [1,2]. Designing a universal driver is challenging because operating conditions vary widely in terms of capacitance, voltage and repetition frequency. This review presents the main pulse generation methods and cooling strategies for modern electro-optic applications.

The main technical challenge in Pockels cell drivers is delivering fast rise and fall times while charging and discharging capacitive loads that typically range from 1 to 100 picofarads [2,3]. At repetition rates in the megahertz range, switching losses and heat buildup become severe. Effective thermal management is essential, as high operating temperatures can reduce efficiency and compromise reliability. Solutions include air cooling by natural or forced convection, solid-state approaches such as heat sinks and thermoelectric devices, liquid-based cooling through immersion or microchannels and phase-change methods including heat pipes and boiling dielectric fluids [4].

Table 1. High-voltage pulse generator architectures comparison

Architecture	Voltage	Frequency	Cost	Size	Complexity	Stability
Vacuum Tubes	Hundreds kV	Few MHz	+++	+++	+++	+
Voltage Multipliers	Tens kV	Few MHz	++	+	+	+
Marx Generator	Hundreds kV	Few MHz	++	++	++	++
Blumlein Structure	Tens kV	Few MHz	++	++	++	+++
PFN	Tens kV	Hundreds kHz	++	++	++	+++
Tesla Transformer	Hundreds kV	Few kHz	++	++	++	++
SMPS	Tens kV	Hundreds kHz	++	++	+++	+++
SS Switches	Tens kV	Tens MHz	+	+	++	++
HV OPAMPs	Few kV	Hundreds kHz	++++	++	+	+

Multiple pulse generation architectures have been explored (see Table. 1). Vacuum tubes could sustain extremely high voltages but were bulky, complex and are now largely obsolete [5]. Voltage multipliers remain compact and simple, though they suffer from voltage drop and ripple when scaled to high frequencies [4]. Marx generators[6] operate by charging capacitors in parallel and discharging them in series. Modern solid-state Marx generators using MOSFETs and IGBTs can achieve nanosecond-scale pulses with excellent scalability and efficiency [6–8]. Blumlein structures produce rectangular, stable pulses but lack flexibility in pulse width [5]. Pulse-forming networks provide flat-top pulses with robust operation but also limited adaptability [5]. Tesla transformers enable resonant high-voltage generation but require precise tuning. Switching-mode power supplies, when combined with multipliers or pulse-forming stages, achieve compact, modular and precisely controlled pulse outputs [4]. Solid-state switches now offer the

best balance of performance. Gallium nitride excels in sub-nanosecond switching with low losses, while silicon carbide provides superior thermal stability and high breakdown voltages [9,10]. High-voltage operational amplifiers exist, but are impractical for nanosecond-scale drivers due to high cost and slow response [5].

When comparing these architectures, vacuum tubes and high-voltage op-amps are considered obsolete or too limited [5]. Blumlein structures, pulse-forming networks, Tesla transformers and voltage multipliers are still relevant for specific use cases where simplicity or pulse shape is more important than versatility [4,5]. The most practical solutions today are based on solid-state switching, switching-mode supply circuits and modern Marx generators [6–10]. Hybrid approaches that integrate GaN or SiC switches with pulse-forming circuits or multipliers provide the best compromise between speed, compactness, stability and cost [7–10].

In conclusion, while classical designs such as vacuum tubes and simple Marx or Tesla circuits remain historically important, they do not meet the compactness, speed and reliability demanded by modern systems [5–7]. The most promising solutions rely on hybrid architectures using wide-bandgap semiconductors, especially gallium nitride and silicon carbide, combined with modular pulse-forming or switching-mode supply stages [9,10]. These technologies are paving the way for next-generation Pockels cell drivers capable of delivering stable, high-voltage, nanosecond pulses for advanced optical and laser applications.

References

1. Zhao, Z. et al. An ultrafast laser pulse picker technique for high-average-current high-brightness photoinjectors.
2. Mittal, S. et al. Design and Development of Pockels Cell Driver for Q Switch LASER in Space Applications.
3. Kim, H.S. et al. Solid-State Pulsed Power Modulator with Fast Rising/Falling Time and High Repetition Rate for Pockels Cell Drivers.
4. Zhuge, Y. et al. Comprehensive Overview of Power Electronics Intensive Solutions for High-Voltage Pulse Generators.
5. Ranjan, A. et al. Review of Nanosecond Pulse Generator with High-Power Switching Devices.
6. Zhong, Z. et al. Review on Solid-State-Based Marx Generators.
7. Wu, F. et al. All-Solid-State Ultrashort Pulse Generator by Capacitive Chopping Circuit. IEEE Trans. Power Electron.
8. Jin, Y. et al. An Inductive Isolation-Based 10 kV Modular Solid Boost-Marx Pulse Generator.
9. Shu, J. et al. A Dynamic Two-Stage Gate Driver for Unlocking the Fast-Switching Potential of GaN HEMT.
10. Ghafoor, S. et al. A Scalable Isolated Gate Driver With Programmable Frequency and Duty Cycle for Series-Connected SiC MOSFETs.

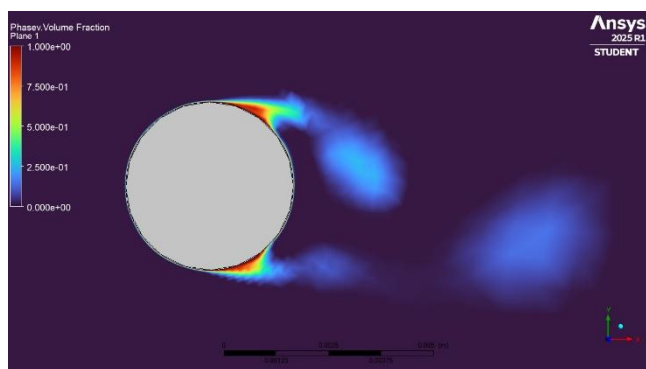
Leidenfrosto garo plėvelės poveikio karšto kūno šilumos perdavimui skaitinis modeliavimas

Mantas Mackelis¹

¹Lietuvos energetikos institutas, Šiluminių įrengimų tyrimo ir bandymų laboratorija
Breslaujos g. 3, LT-44403 Kaunas, el. p.: Mantas.Mackelis@lei.lt

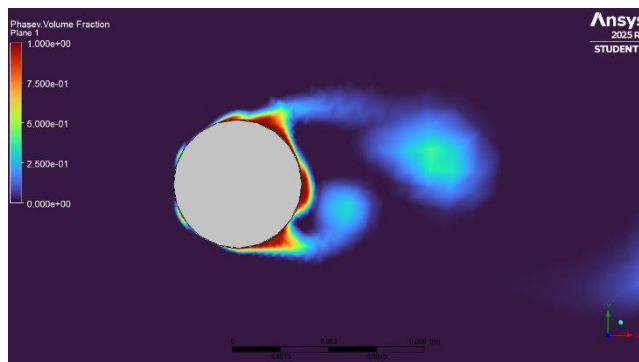
Leidenfrosto reiškinys lemia stabilios garo plėvelės susidarymą ant perkaitinto paviršiaus, dėl ko drastiškai krinta šilumos perdavimo koeficientas ir skysčiui tekant sumažėja kūno aerohidrodinaminis pasipriešinimas. Skaitmeninis prognozavimas vis dar kelia iššūkių dėl daugiafazio fronto sekimo ir fazių kaitos modelių parametrizacijos. Šio darbo tikslas – ANSYS aplinkoje sukurti daugiafazį (VOF) modelį su Lee garavimo/kondensacijos koeficientais ir k- ω SST turbulencijos modeliu, leidžiantį prognozuoti garo plėvelės stabilumą bei šilumos perdavimo koeficiento kaitą. Tyrimo objektas – varinis kamuoliukas vandens sraute.

Modeliavimas atliktas ANSYS Fluent aplinkoje taikant VOF daugiafazį metodą garo–skysčio sąsajai sekti ir Lee garavimo/kondensacijos modelį fazių kaitai aprašyti. Turbulencijai naudotas k- ω SST modelis. Geometrija: varinis kamuoliukas $D = 19$ mm tiesinio kanalo centre. Skaitinis tinklėlis -sieniniame sluoksnyje 25 augančių sluoksnių (augimo koef. = 1,2, pirmo sluoksnio storis = 0.005 mm). Įtekėjimas: $U = 1,9$ m/s, $T_{\text{skysčio}} = 293$ K, vienfazis vanduo; išteklėjimas – slėgio sąlyga (0 Pa). Kamuoliuko paviršiuje taikyta pradinės temperatūros sąlyga $T_{\text{kūno}} = 473$ K ir no-slip. Lee koeficientai parinkti literatūriniu intervalu ir kalibruoti plėvelės stabilumo bei šilumos srauto atkartojimui ($S_{\text{evap}} = 600 \text{ s}^{-1}$; $S_{\text{cond}} = 30 \text{ s}^{-1}$). Pritaikytas adaptyvus laiko žingsnis $\Delta t \approx 1 \cdot 10^{-6} \text{ s}$ su Couranto skaičiumi $< 0,5$. uždavinys spręstas pereinamosios būsenos režimu (transient).



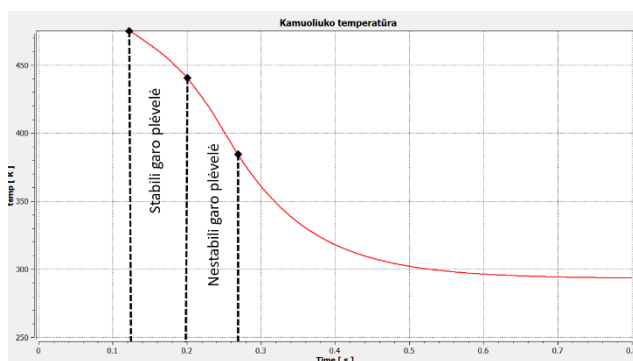
1 pav. Modelis su stabilia garo plėvele.

Pereinamosios būsenos skaičiavimai parodė - stabilios garo plėvelės išsilaikė $t \approx 0,07$ s; plėvelė žlugo, kai kamuoliuko paviršius atvėso nuo $T_0 = 473$ K iki $T \approx 440$ K.



2 pav. Garo plėvelės žlugimas.

Po žlugimo prasidėjo nukleacija, dėl kurios šilumos perdavimas reikšmingai išaugo, ir kūnas per papildomas $\sim 0,9$ s (viso $\sim 0,16$ s nuo pradžios) pilnai atvėso iki vandens virimo temperatūros ($T \approx 373$ K, 1 atm).



3 pav. Kamuoliuko temperatūros kitimas laike.

3 pav. pavaizduota kamuoliuko temperatūra $T(t)$ vandenyje ($D = 19$ mm, $U = 1,9$ m/s, $T_0 = 473$ K). Garo plėvelė stabili iki $t \approx 0,19$ s ($T \approx 441$ K), po žlugimo prasideda nukleacija iki $t \approx 0,28$ s, T pasiekia vandens virimo temperatūrą (373 K). Vertikalios linijos žymi stabilios ir nestabilios plėvelės režimus. Stabilios plėvelės režime temperatūra kinta lėtai, o plėvelei žlugus temperatūros kritimas suintensyvėja.

Literatūra

- Natalia Holešova, Richard Lenhard, Katarina Kaduchova, Milan Malcho, Correlation Coefficients in Lee's Model of Multiphase Flows (Slovakia, 2022).
- Ivan U. Vakarelski, Farrukh Kamoliddinov, Aditya Jetly, Sigurdur T. Thoroddsen, Leidenfrost spheres, projectiles, and model boats: Assessing the drag reduction by superhydrophobic surfaces (Saudi Arabia, Bulgaria, 2024).
- David Quéré, Leidenfrost Dynamics (France, 2012).

Investigation of New Electron-Transporting Materials in Perovskite Solar Cells Using the Kinetic Photoconductivity Method

Dovilė Vasiliauskaitė¹, Lauryna M. Svirskaitė², Vidmantas Gulbinas¹, Ernestas Kasparavičius¹

¹Center for Physical Sciences and Technology, Department of Molecular Compounds Physics
Saulėtekio av. 3, LT-10257 Vilnius, email: dovile.vasiliauskaite@ftmc.lt

²Kaunas University of Technology, Faculty of Chemical Technology, Department of Organic Chemistry, Radvilėnų av. 19, LT-50254 Kaunas

In the modern world, the demand for electricity derived from renewable energy sources, such as solar radiation, wind, hydropower, and geothermal energy, is steadily increasing. This growing interest in environmentally sustainable energy solutions has driven rapid progress across many technological fields, with photovoltaic (PV) devices standing out as a particularly dynamic area of development.

Over the past decade, perovskite solar cells (PSCs) have attracted remarkable scientific attention within photovoltaic research. From 2009 to 2024, the power conversion efficiency (PCE) of perovskite-based solar cells has risen from only 3.8% to 26.1% [1,2]. This rapid growth in performance, along with the technological appeal of perovskites, is largely attributed to their favourable physical properties, such as high charge-carrier mobility and long diffusion lengths, combined with relatively simple fabrication methods, a tunable bandgap, and innovative device architectures. Equally important is a deeper understanding of the fundamental physical processes that govern device performance, including recombination dynamics, lattice and interface defects, charge generation, transport, and their mutual interactions.

In this work we investigate how different synthesized organic compounds, used as electron transport layers (ETLs), influence charge-carrier dynamics in perovskite solar cells by using the kinetic photoconductivity method.

The solar cell samples were fabricated via the spin-coating method. Samples were prepared and mounted in a customized holder. The devices were excited using a laser and measurements were taken under various illumination intensity conditions. Additionally, standard photovoltaic characterisation was performed to evaluate device parameters, such as PCE values.

Based on the experimental results, our study examines how the selected organic compounds affect the photoconductivity of perovskite solar cells. From these observations an approximate energy-level alignment diagram was constructed.

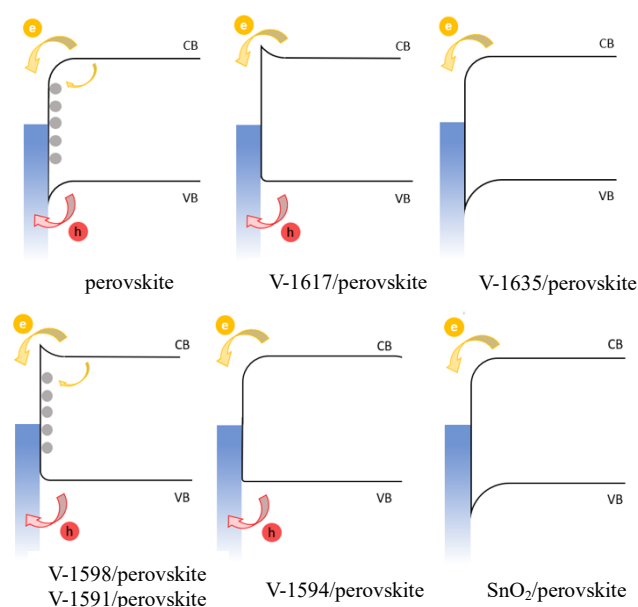


Figure 1. Approximate energy band diagram for different solar cells.

References

1. S. Bhattarai, A. Mhamdi, I. Hossain, et. al, A detailed review of perovskite solar cells: Introduction, working principle, modelling, fabrication techniques, future challenges, Micro and Nanostructures, 172, 2773-0123, 2022.
2. Jiarong Wang, Leyu Bi, Qiang Fu, Alex K.-Y. Jen, Methods for Passivating Defects of Perovskite for Inverted Perovskite Solar Cells and Modules, Advanced energy materials, 14 (35), 2401414, 2024.

PRIVERSTINĖS BRILIUENO SKLAIDOS LAZERIO IMPULSŲ SPAUSTUVAS NAUDOJANT HT-230 SKYSTĮ

Rugilė Pečiulytė¹, Paulius Mackonis¹, Aleksėj Rodin¹, Augustė Černeckytė¹

¹Fizinių ir technologijos mokslų centras, Lazerinių technologijų skyrius
Savanorių pr. 231, LT-02300 Vilnius, el. p.: rugile.peciulyte@ftmc.lt

Didelės energijos pikosekundinių lazerių paklausa sparčiai auga. Tokie lazeriai turi plačias taikymo galimybes nuo lazerinės palydovų nuotolinės detekcijos ir lazerinės kosmetologijos iki didelio našumo medžiagų apdirbimo. Vis dėlto, įprasti pikosekundinių lazerio impulsų generavimo metodai yra riboti. Kokybės moduliacijos būdu generuojami sub-ns trukmės impulsai, o modų sinchronizacija užtikrina tik mažą išvadinę impulsų energiją. Kita vertus, sub-ns impulsai lazeriniame apdirbime sukelia šiluminę pažeidą, o maža energija nėra tinkama didelių plotų apdirbimui. Nors didelės energijos pikosekundiniai impulsai gaunami naudojant brangesnius spinduolių–stiprintuvų (MOPA, angl. master-oscillator power amplifier) sistemas, tokiu atveju dažnai nukenčia išvadinio pluošto kokybę. Todėl mažos savikainos, didelės energijos pikosekundinių lazerių kūrimas, užtikrinant aukštą pluošto kokybę, vis dar kelia nemažai iššūkių.

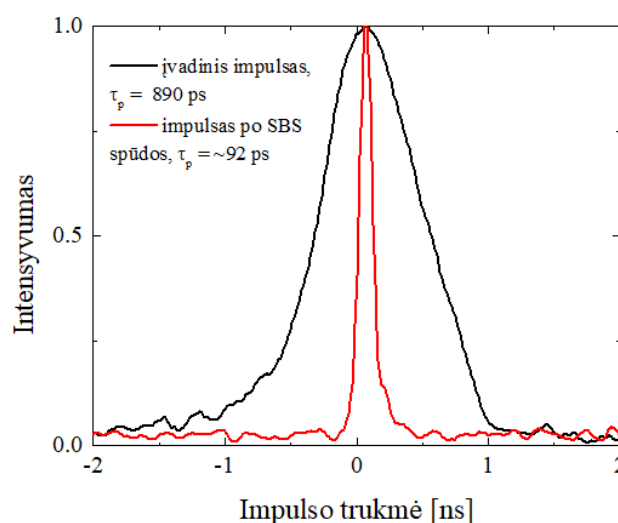
Alternatyva - impulsų spūda taikant priverstinę Briliueno sklaidą (SBS, angl. stimulated Brillouin scattering), naudojant palyginti nebrangius pasyvios kokybės moduliacijos nanosekundinius lazerius. SBS bangos fronto apgrąžos veidrodis leidžia pagerinti pluošto kokybę, kompensuojant bangos fronto iškreipimus, kuriuos sukelia optiniai elementai pluošto sklaidimo ir stiprinimo metu.

Ankstesniuose tyrimuose SBS-aktyviose terpėse impulsai buvo suspausti iki ~70 ps anglies tetrachloride (CCl_4) [1] ir iki ~90 ps perfluoroktane (C_8F_{18}) [2]. Šiame darbe panaudotas HT-230 skystis, pasižymintis itin trumpu akustinių fononų gyvavimo laiku [3] ir aukštu optinės pažeidos slenksčiu. Tyrimo tikslas buvo ištirti įvairias SBS-spaustuvo konfigūracijas su HT-230 skysčiu, naudojant nanosekundinį kokybės moduliacijos lazerį. Buvo tiriama SBS impulsų spūda naudojant skirtingo židinio nuotolio fokusuojančius lęšius, siekiant nustatyti optimalias veikimo sąlygas bei palyginti SBS spūda HT-230 ir C_8F_{18} skysčiuose. Trymo metu pasiekta maksimali impulsų spūda iki ~90 ps ir ~110 trukmės atitinkamai HT-230 ir C_8F_{18} skysčiuose.

Eksperimente naudota dviejų lėkių stiprintuvo schema. Užkrato šaltinis – kompaktiškas pasyvios kokybės moduliacijos Nd:YAG lazeris (UAB „QS Lasers“), generuojantis 1064 nm bangos ilgio, 1.6 mJ energijos, ~0.9 ps trukmės impulsus 10 Hz dažniu. Užkrato spinduliuotė buvo stiprinama dviejuose šoninio diodinio kaupinimo Nd:YAG kristalo stiprintuvuose iki ~6 mJ, bei fokusuojama į SBS kiuvetę. SBS-spūda vyko 35 cm ilgio kiuvetėje, pripildytoje nanofiltru išvalytu HT-230 arba C_8F_{18} skysčiu. Atspindėtas SBS impulsas dar kartą stiprintas Nd:YAG stiprintuve.

SBS atspindžio koeficiento ir impulsų trukmės matavimai parodė, kad HT-230 skystyje didžiausias SBS atspindys (~40%) ir minimali SBS Stokso impulso

trukmė (~90 ps) pasiekti naudojant $f = 250$ mm lęšį ir esant 5,8 mJ įvadinei impulsų energijai (1 pav.). C_8F_{18} skystyje šiomis sąlygomis pasiektas didesnis SBS atspindžio koeficientas (~50%), tačiau lazerio impulsas suspaustas tik iki ~110 ps. SBS spūdos HT-230 skystyje atspindžio pluoštas taip pat pasižymėjo itin pagerinta kokybe lyginant jį su užkrato lazerio pluoštu: SBS pluošto kokybė ($M^2 = 1,2$, kai pradinė užkrato lazerio pluošto kokybė $M^2 \approx 2$).



1 pav. Įvadinis ir Stokso impulsai optimaliomis SBS-spūdos sąlygomis HT-230 skystyje, τ_p – impulso trukmė pusaukštyje.

Tolimesniuose tyrimuose planuojama panaudoti „savaiminio užkrato“ SBS metodą, leidžiantį sumažinti slenksį, pasinaudojant Stokso komponentu atspindėtame pluošte, taip pat pagerinti energijos stabilumą, sumažinti laikinį nestabilumą (angl. jitter) ir pasiekti trumpesnius impulsus [1,2]. Todėl SBS-spaustuvas, ypač integruotas su keturių lėkių stiprintuvu, gali būti kompaktiškas ir efektyvus sprendimas didelės energijos pikosekundiniams impulsams generuoti.

Suspausti didelės energijos pikosekundiniai impulsai su puikia pluošto kokybe gali būti pritaikyti lazerinėje dermatologijoje, ypač šalinant tatuiruotes, taip pat didelio našumo funkcinių medžiagų gamybai, naudojant interferencinę abliaciją.

SBS-spūda, priverstinė Briliueno sklaida, anglies tetrachloridas, perfluoroktanas.

Literatūra

1. A.S. Dement'ev, I. Diomin, E. Murauskas, N. Slavinskis, Quantum Electronics **41** (2011).
2. A.M. Rodin, A. Černeckytė, P. Mackonis, A. Petrušėnas, Photonics **10**, 1060 (2023).
3. Y. Chen, B. Tan, D. Jin, et al., High Power Laser Science and Engineering **12**, 10 (2024).

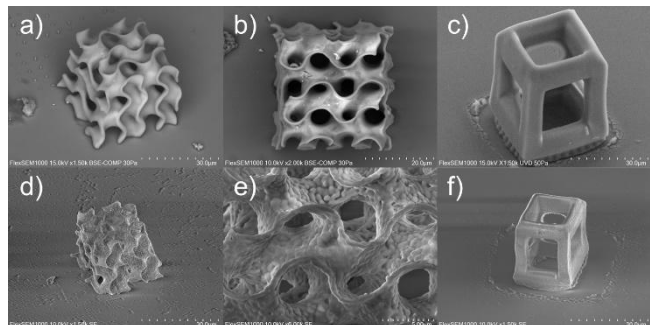
YAG:Ce³⁺ 3D mikrostruktūrų gamyba naudojant dvifotonę polimerizaciją ir kalcinaciją

Robertas Virkėtis¹, Artūr Harnik², Dominykas Dapšys², Dimitra Ladika², Greta Merkininkaitė¹, Simas Šakirzanovas¹, Mangirdas Malinauskas²

¹Vilniaus universitetas, Chemijos ir geomokslų fakultetas, Chemijos institutas
Naugarduko g. 24, LT-03225 Vilnius, el. p.: robertas.virketis@chgf.vu.lt

²Vilniaus universitetas, Fizikos fakultetas, Lazerinių tyrimų centras
Saulėtekio al. 10, LT-10223 Vilnius

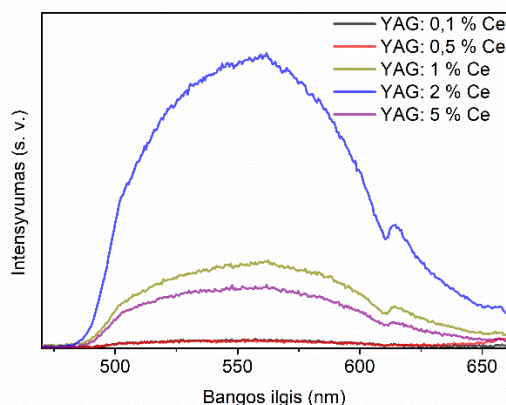
Itrio aliuminio granatai (YAG) pasižymi dideliu kietumu, stabilumu aukštose temperatūrose bei optiniu pralaidumu regimajai šviesai [1] ir dėl šių savybių jau 60 metų yra naudojami, kaip lazerių aktyvioji terpė [2]. YAG monokristalų pagrindinis gamybos būdas yra Čochralskio metodas, o pilokristaliniais YAG gauti, dažniausiai yra naudojami zolių-gelių metodas, kietfazė sintezė, karštasis izostatinis presavimas ir vakuuminis sukepinimas. Tačiau ne vienas iš šių būdų nėra tinkamas laisvos formos kristalinių 3D mikrostruktūrų gamybai. Daugiafotonės polimerizacijos metodas leidžia atspausdinti mikrometrų eilės polimerinius 3D darinius, kuriuos termiškai apdorojant yra gaunami keraminiai dariniai [3]. Šiuo darbu yra parodoma, kad naudojant dvifotonę polimerizaciją ir supolimerizuotų 3D darinių kalcinaciją galima pagaminti YAG:Ce³⁺ 3D mikrostruktūras, pasižyminčias liuminescencinėmis savybėmis [4].



1 pav. Dvifotonės polimerizacijos metodu atspausdinti polimeriniai 3D mikrodariniai: a) gyroidas, b) gyroido vaizdas iš viršaus, c) kubinė gardelė. Ir YAG:Ce³⁺ 3D mikrostruktūros po kalcinacijos 1600 °C: d) gyroidas e) gyroido vaizdas iš viršaus, f) kubinė gardelė.

YAG:Ce³⁺ pirmtakų polimerinės 3D mikrostruktūros buvo pagamintos naudojant dvifotonės polimerizacijos metodą ir „NanoFactory“ (UAB „Femtika“) femtosekundinio lazerio litografinę sistemą. Spausdinimui buvo naudotas 517 nm antrosios harmonikos bangos ilgis ir 144 fs impulsų lazeris. Norint nustatyti optimalius spausdinimo parametrus darinių gamybai, buvo spausdinami „narvų“ masyvai keičiant skenavimo greitį ir spinduliuotės galią. Mėginiai po polimerizacijos buvo ryškinami organiniame tirpiklyje etanolyje, pašalinant nesupolimerizuotą dervą. Po ryškinimo polimeriniai 3D mikroobjektai buvo kalcinuojami trim etapais. Pirmiausia ore 1000 °C temperatūroje su 1 valandos išlaikymu, pašalinant organinę dalį. Po to 1600 °C temperatūroje išlaikant 1 valandą ore, suformuojant gryną Y₃Al₅O₁₂ kristalinę fazę. Ir galiausiai redukcinėje

atmosferoje (95 % N₂ + 5 % H₂) išlaikant 1 valandą 1000 °C, suredukuojant Ce⁴⁺ iki Ce³⁺, taip pagerinant darinių liuminescencines savybes. Monokristalinės rentgeno spindulių difrakcinės analizės metodas patvirtino, kad po kalcinacijos gaunami 3D mikrodariniai yra vienfaziai gryni Y₃Al₅O₁₂. YAG:Ce³⁺ 3D mikrostruktūrų liuminescencijos matavimų metu sužadinimui buvo naudojama 450 nm bangos ilgio spinduliuotė. Nustatyta, kad pagaminti 3D mikroobjektai iškaitinti 1600 °C pasižymi liuminescencinėmis savybėmis, o jų emisijos juostos maksimumas yra ties 560 nm. Intensyviausia emisija pasižymėjo YAG:Ce³⁺ mikrostruktūra, kurios legiravimo laipsnis yra 2 %.



2 pav. YAG legiruoto 0,1 %, 0,5 %, 1 %, 2 %, 5 % Ce³⁺ 3D mikrodarinių (iškaitintų 1600 °C) emisijos spektrai (sužadinimui naudotas 450 nm bangos ilgis).

Padėka

Šis tyrimas buvo atliktas pagal Lietuvos Respublikos švietimo ir mokslo ministerijos programą „Universitetų meistriškumo iniciatyva“ („Universities Excellence Initiative“) pagal sutartį su Lietuvos mokslo taryba (projekto Nr. S-A-UEI-23-6) ir finansuotas Vilniaus universiteto Mokslo skatinimo fondo (projekto Nr. MSF-JM-10/2024).

Literatūra

1. Y. Zhang, J. Liu, Y. Zhang, H. Yang, Y. Yu, Q. He, X. Liang, Y. Liu, W. Xiang, J. Alloys Compd. **488**, 638-642, (2009).
2. Zac, “Is It Time To Invest In A Cutera YAG Laser?”, laserresell, May 16 2022, <https://laserresell.com/buying-used-equipment/cutera-yag-laser/>, (Accessed: 28 August 2025).
3. Skliutas, E., Merkininkaitė, G., Maruo, S. et al. Multiphoton 3D lithography. *Nat Rev Methods Primers* **5**, 15 (2025).
4. A. Harnik and et. Al., „Laser 3D micro-/nano-structurization of luminescent materials”, *Adv. Opt. Mater.* **13**, 25000316 (2025).

INVESTIGATION OF SPECTROSCOPIC PROPERTIES OF FREE-BASE TETRAPHENYLPORPHYRIN AND HEXAGONAL BORON NITRIDE VAN DER WAALS COMPLEX

Jelizaveta Fedotova^{1,2}, Martynas Talaikis¹, Patrizia Lamberti³, Jevgenij Chmeliov^{1,2}, Maksim Shundalau^{3,4}, Renata Karpicz¹, Ivan Halimski¹

¹Center for Physical Sciences and Technology, Department of Molecular Compound Physics
Saulėtekio av. 3, LT-10257 Vilnius, email: jelizaveta.fedotova@ftmc.lt

²Vilnius University, Faculty of Physics
Saulėtekio av. 9-III, LT-10222 Vilnius

³University of Salerno, Department of Information and Electrical Engineering and Applied Mathematics
via Giovanni Paolo II 132, 84084 Fisciano, Italy

⁴University of Warsaw, Faculty of Physics
ul. Pasteura 5, 02-093 Warsaw, Poland

Two-dimensional (2D) hexagonal boron nitride (hBN) attracts significant interest due to its specific properties and wide scope of applications. It is isoelectronic to graphene, however, in contrast to latter, it is an electronic insulator. It has high chemical and thermal stability as well as high thermal conductivity. hBN can be applied in optoelectronics, in photonics and imaging; it has already been applied as dielectric layer in field effect transistor. Downsizing the 2D hBN allows to obtain 0D hBN quantum dots, which are biocompatible and, thus, can be used as a platform for target drug delivery.

To widen the scope of hBN applications it is important to understand how it interacts with different compounds. One of the possible and promising interactions is weak van der Waals (vdW) interaction between hBN and another compound, because it allows to modify physical and chemical properties of the compounds without violating their structures. For example, recently it was shown that hBN can form vdW complex with *trans*-stilbene [1] and the manifestation of the interaction can be observed in THz, IR and visible regions.

In this study we investigated optical properties of vdW complex formed between hBN and tetraphenylporphyrin (TPP) with Raman, IR absorption as well as with UV/vis absorption and steady-state fluorescence (FL) and FL decay kinetics. We observed, that Raman bands assigned to the phenyl rings of TPP exhibit blue shifts in the spectrum of the complex with respect to the pure TPP, while TPP macrocycle bands exhibit red shifts in the complex. All bands in UV/vis spectra and steady-state FL exhibit notable red shifts in the spectrum of the complex. These bands are also associated with changes in macrocycle geometry upon electronic excitation. The same tendencies for another porphyrin compound were recently published by Korolkov, et.al [2]. Additional feature of the complex between TPP and hBN is reduced quenching of FL decay in the complex with respect to pure TPP.

References

1. I. Halimski, et. al., Langmuir 41, 11, 7364 (2025).
2. V.V. Korolkov, et.al., ACS Nano 9, 10, 10347 (2015).

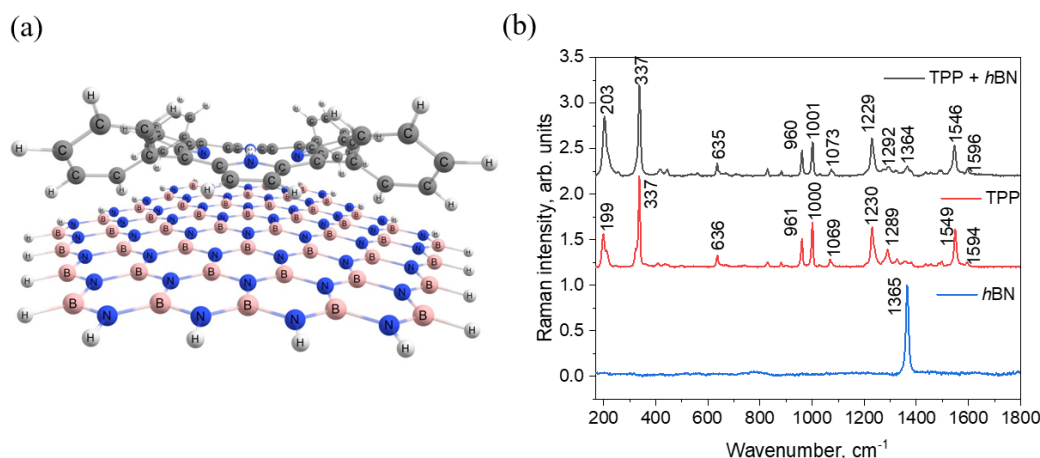


Figure 1. a) Optimized geometry of TPP + hBN complex and b) Raman spectra of TPP + hBN, TPP and hBN

Charge Carrier Dynamics at the Perovskite/Graphene–MoO₃ Interface

Noor ul Ain Ahmed¹, Georgy Fedorov², Polina Kuzhir², Renata Karpicz³ Ernestas Kasparavičius³
Vidmantas Gulbinas³ Patrizia Lamberti¹

¹Department of Information and Electrical Engineering and Applied Mathematics, University of Salerno
Fisciano (SA), Italy. Email: nahmed@unisa.it

²Department of Physics and Mathematics, Faculty of Science, Forestry and Technology, University of Eastern Finland
Joensuu, Finland

³Department of Physics of Molecular Structures, Center for Physical Sciences and Technology
Vilnius, Lithuania.

Understanding charge carrier dynamics at perovskite interfaces is essential for improving the performance and stability of next-generation optoelectronic devices. Interface engineering plays a key role in controlling charge extraction, recombination, and ion migration processes [1]. This work investigates charge carrier dynamic at the interface between hybrid CsMAFA based perovskite films and graphene–MoO₃ hole-collecting contacts using a capacitive device structure designed to block electron extraction [2]. The configuration allows selective analysis of hole transport and recombination dynamics through transient photovoltage measurements under illumination. Measurements were performed under dark, illuminated, and saturated conditions, and recorded at successive time intervals to study the evolution of photovoltage with illumination history. The results reveal illumination-dependent changes in the transient response, indicating persistent memory effects within the perovskite layer. These time-resolved observations highlight the role of interfacial electric fields, charge trapping and recombination, and charge accumulation in governing potential dynamics. Overall, the graphene–MoO₃ contact exhibits efficient hole collection, demonstrating its promise as a transparent electrode for probing and optimizing charge carrier dynamics in perovskite-based devices.

Acknowledgment

This work was partially supported by the EU under the Italian National Recovery and Resilience Plan (NRRP) of NextGenerationEU, Project Title UPWARD CUP E53D23014490001 - Grant Assignment Decree No. 1383 of 01/09/2023, by partnership on “Telecommunications of the Future” (PE00000001 - program “RESTART”) and from the Horizon Europe MSCA programme under FLORIN project (GA n° 101086142).

References

1. H. Tong et al., ‘Interface Engineering, Charge Carrier Dynamics, and Solar-Driven Applications of Halide Perovskite/2D Material Heterostructured Photocatalysts’, ACS Applied Materials & Interfaces, vol. 17, no. 16, pp. 23431–23465, 2025, doi: 10.1021/acsami.4c20972.
2. E. Kasparavičius, M. Franckevičius, S. Driukas, and V. Gulbinas, ‘Charge Carrier Dynamics at the Perovskite Interface with Self-Assembled Monolayers’, ACS Applied Materials & Interfaces, vol. 16, Oct. 2024, doi: 10.1021/acsami.4c10223.

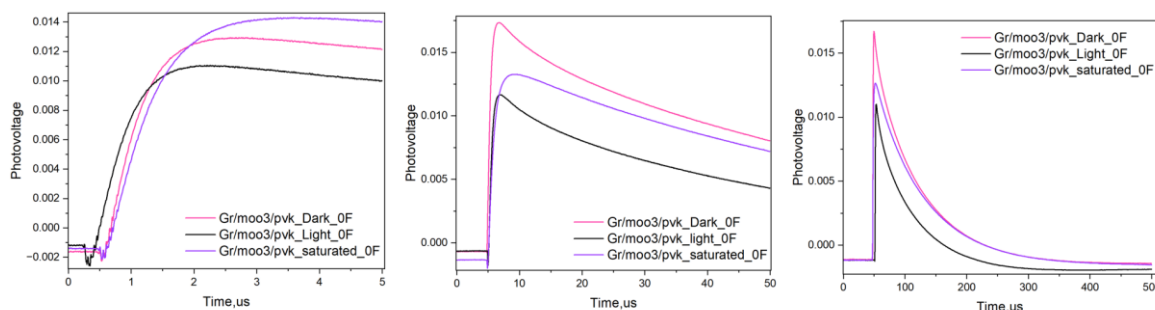


Figure 1. Transient photovoltage of the Graphene/MoO₃/Perovskite device under dark, light, and saturated conditions, showing illumination-dependent variations in amplitude and decay behavior

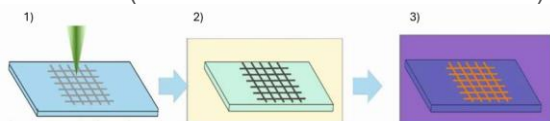
Elektrochrominių sluoksnių ir skaidrių vario takelių elektrodų spektrinis tyrimas

Titas Tamošauskas¹, Dainius Balkauskas¹, Alexandr Belosludtsev¹

¹Fizinių ir technologijos mokslų centras, lazerinių technologijų skyrius
Savanorių al. 231, LT-02300 Vilnius, el. p.: titas.tamosauskas@ftmc.lt

Auganti energijos paklausa ir ekologiniai iššūkiai skatina diegti technologijas, kurios mažina pastatų energijos suvartojimą. Viena perspektyviausių krypčių – elektrochrominiai „išmanieji langai“, kurių optinės savybės gali būti valdomos elektriniu signalu. Keičiant įtampą, galima reguliuoti UV ir IR šviesos spinduliuotės patekimą į patalpas.

Naudojant lazeriu aktyvuoto paviršiaus metalo nusodinimo technologiją (angl. SSAIL), buvo sukurta skaidrių mikrostruktūrinių metalinių elektrodų gamybos metodika ant stiklo [1]. Tokie elektrodai gali tapti alternatyva dažnai naudojamiems ITO elektrodams, kurie yra brangūs ir kenksmingi aplinkai. Ši metodika susideda iš 3 etapų: 1) Femtosekundiniu impulsiniu lazeriu paruošiamas elektrodų nusodinimo paviršius; 2) Cheminė aktyvacija kataliziniame tirpale sužadintose vietose; 3) Autokatalizinis cheminis metalo nusodinimas (be išorinio elektros srovės šaltinio).



1 pav. SSAIL elektrodų gaminimo etapai

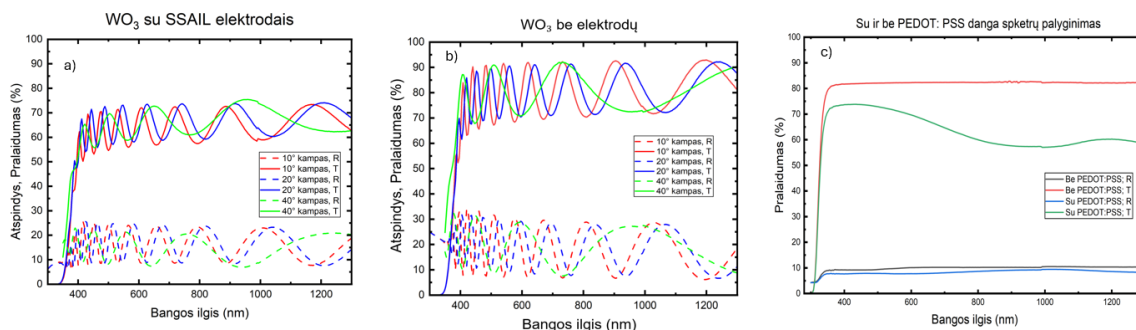
Šiame tyrime yra nagrinėjamos SSAIL elektrodų bei dažnai naudojamų elektrochrominių dangų (WO_3 ir PEDOT:PSS) kombinacijos. WO_3 dangos nusodintos magnetroniniu dulkinimu ant pakreiptų optinių padėklų, kurių kampai yra 10° , 20° ir 40° siekiant porėtesnės struktūros, geresniam jonų transportavimui [2]. Buvo ištirti pralaidumo ir atspindžio spektrai: mėginių su skaidriais elektrodais, suformuotais SSAIL metodu, ir mėginių, sudarytų tik iš elektrochrominės WO_3 dangos.

Nustatyta, kad bandiniai be SSAIL elektrodų (tik WO_3) pasižymėjo didesniu šviesos pralaidumu (68–92 %), būdingu šiai medžiagai. Bandinių su SSAIL elektrodais pralaidumo reikšmės siekė nuo 54 % iki 74 %, bendras pralaidumas buvo mažesnis dėl papildomo šviesos sklaidos, kurį sukelia SSAIL elektrodų mikrostruktūra. Didinant optinio padėklo pakrypimo kampą, spektrai tapo lygesni, o tai siejama su porėtos mikrostruktūros susiformavimu, pagerinančiu optinį moduliavimą dėl interferencijos savybių.

Papildomai buvo ištirti bandiniai su PEDOT:PSS elektrochromine danga. 2 pav. c) pateikti pralaidumo ir atspindžio spektrai suformuotiems mėginiams su ir be PEDOT:PSS sluoksnio. Nustatyta, kad PEDOT:PSS padengti bandiniai pasižymi mažesniu bendru šviesos pralaidumu (58–72 %), lyginant su mėginiais be šios dangos (82–85 %). Šis skirtumas siejamas su papildomu šviesos sugėrimu polimerinėje dangoje, ypač ilgesnių bangų ruože (>700 nm), kur pastebimas nuoseklus pralaidumo mažėjimas. Atspindžio reikšmės abiem atvejais išliko panašios (5–10 %).

Literatūra

- [1] M. Sadauskas, V. Vrubliauskaitė, E. Kvietkauskas, D. Balkauskas, R. Trusovas, A. Belosludtsev, K. Ratautas, Microscale copper traces by laser induced copper deposition on glass and PET substrate, Opt. Laser Technol. 161 (2024)
- [2] R. Misra, R.S. Ajimsha, H.S. Mavi, Electrochromic behavior of WO_3 thin films prepared by glancing angle deposition, Appl. Surf. Sci. 456 (2018) 384–391.



2 pav. WO_3 dangų pralaidumo spektrai su elektrodais (a) ir be elektrodų (b) pralaidumo ir atspindžio spektrai

Microfluidic Preparation of Chitosan Nanoparticles for Drug Delivery

Samanta Gelumbickytė¹

¹Center for Physical Sciences and Technology, Department of Functional Materials and Electronics
Saulėtekio av. 3, LT-10257 Vilnius, email: samanta.gelumbickyte@ftmc.lt

Chitosan nanoparticles have gained significant attention as biocompatible and biodegradable carriers for controlled drug delivery [1]. In this study, a microfluidic approach was employed to synthesize chitosan nanoparticles. Controlled flow, optimized pH, reagent concentrations, and efficient mixing in the microchannel ensured homogeneous reaction conditions during ionic gelation between chitosan and sodium tripolyphosphate (TPP) [2]. Dynamic light scattering (DLS) analysis revealed that the microfluidic method produced nanoparticles with narrow size distribution and positive surface charge, suitable for loading and sustained release of drug molecules. Compared to conventional batch synthesis, the microfluidic approach provided improved reproducibility, scalability, and reduced reagent consumption. These results demonstrate that microfluidic technology offers an efficient and tunable platform for producing polymer-based nanocarriers. The developed system can be further optimized for encapsulating various therapeutic agents, presenting a promising route toward advanced and targeted drug delivery applications.

References

1. K. Jaferník, A. Ładniak, E. Blicharska, K. Czarnek, H. Ekiert, A.E. Wiącek, and A. Szopa, *Molecules* 28, 1963 (2023).
2. H. Zhang, J. Yang, R. Sun, S. Han, Z. Yang, and L. Teng, *Acta Pharm. Sin. B* 13, 3277 (2023).

ENHANCED PERFORMANCE OF GOLD NANOPARTICLES MODIFIED NICKEL-IRON FOR SODIUM BOROHYDRIDE OXIDATION

Dmytro Shyshkin¹

¹Fizinių ir technologijos mokslų centras, Katalizės skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: dmytro.shyshkin@ftmc.lt

Hydrogen-rich compounds, including sodium borohydride (NaBH_4), which possesses a substantial hydrogen content of 10.6 wt% and an energy density of 9.3 Wh g^{-1} [1], have emerged as a compelling candidate for carbon-free energy applications. NaBH_4 has been the focus of extensive research as a prospective fuel for direct borohydride fuel cells (DBFCs), which possess a high theoretical cell voltage of 1.64 V [2,3]. DBFC functions through two fundamental half-cell reactions: the anodic half-reaction involves the borohydride oxidation reaction (BOR), while the cathodic half-reaction corresponds to the oxygen reduction reaction (ORR). The BOR generally exhibits a high overpotential, which considerably restricts the output voltage of DBFCs. Therefore, it is imperative to rationally design BOR electrocatalysts to enhance their catalytic performance in order to optimize the overall efficiency of these fuel cells.

In this study we present a strategy to fabricate flexible electrocatalysts based on Ni-Fe coatings modified with AuNPs. As flexible substrate we use polyimide which is lightweight, flexible, resistant to heat and chemicals. MB was chosen as a reducing agent for depositing the NiFe coating because it is a relatively mild, stable, and less explosive, toxic, and environmentally friendly alternative to traditional reducing agents like hydrazine (N_2H_4) or NaBH_4 . The deposited NiFe coatings on the copper-coated polyimide were additionally modified with AuNPs through galvanic displacement to enhance their electrocatalytic performance in NaBH_4 electrooxidation. Scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), and inductively coupled plasma optical emission spectroscopy (ICP-OES) were used to examine the structural and morphological characteristics of the coatings, confirming the formation of a NiFe alloy matrix and the presence of dispersed AuNPs (Fig. 1). Electrochemical characterization, including cyclic voltammetry, demonstrated that the AuNPs-modified NiFe coatings exhibited significantly enhanced catalytic performance, characterized by higher current densities, lower onset potentials, and reduced charge transfer resistance, compared to the unmodified NiFe coating. Further evaluation in a DBHPFCs configuration revealed that the AuNPs-NiFe anode exhibited a superior power density of 89.7 mW cm^{-2} at room temperature and demonstrated operational stability under alkaline conditions, whereas the NiFe anode exhibited a power density of 73.1 mW cm^{-2} (Fig. 2) This enhanced performance is attributed to the synergistic interaction between the highly active AuNPs and the conductive NiFe matrix, which promote efficient borohydride oxidation and electron transfer collectively.

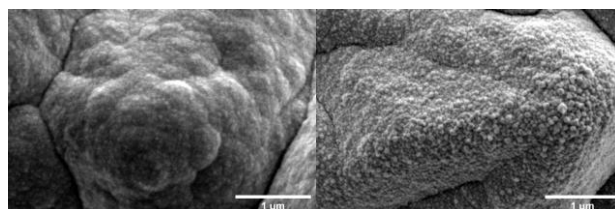


Figure 1. SEM images of the NiFe (a) and AuNPs-NiFe (b) catalysts deposited on the Cu/PI surface.

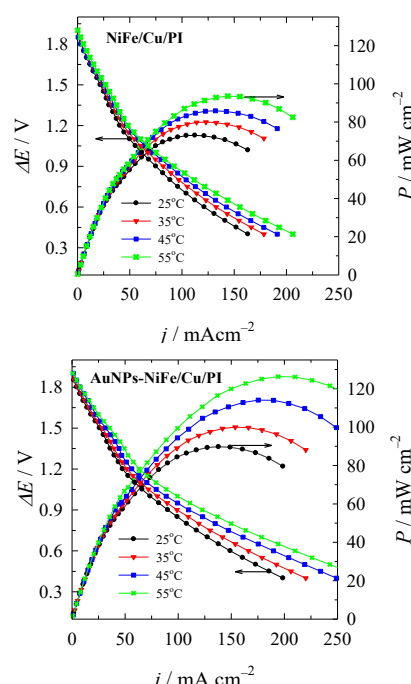


Figure 2. Cell polarization and power density curves for the direct $\text{NaBH}_4\text{-H}_2\text{O}_2$ fuel cell using NiFe/Cu/PI (a) and AuNPs-NiFe/Cu/PI (b) catalysts as the anodes/cathodes using the anolyte consisting of 1 M NaBH_4 and 4 M NaOH and the catholyte consisting of 5 M H_2O_2 and 1.5 M HCl at different temperatures.

This work presents a novel, cost-effective, and highly active anode engineering strategy for DBHPFCs with a focus on NiFe-based materials modified with a noble metal for use in electrocatalytic NaBH_4 electrooxidation and other hydrogen-based energy systems.

References

1. B. He, S. Zhuang, X. Tai, et al. ACS Appl. Mater. Interfaces 14(15), 17631 (2022).
2. X. Yin, Q. Wang, D. Duan, S. Liu and Y. Wang. Int. J. Hydrogen Energy 44(21), 10971 (2019).
3. G. Braesch, Z. Wang, S. Sankarasubramanian, A.G. Oshchepkov, A. Bonnefont, E. R. Savinova, V. Ramani and M. Chatenet. J. Mater. Chem. A 8(39), 20543 (2020).

FORMATION OF CHANNELS IN SODA-LIME GLASS USING A LASER ABLATION AND CHEMICAL ETCHING THROUGH A THIN CHROMIUM LAYER MASK

Daumantas Sriubas¹

Center for Physical Sciences and Technology, Department of Laser research
Savanorių ave. 231, LT-02300 Vilnius, email: daumantas.sriubas@ftmc.lt

Glass micropatterning is important in many novel technologies, such as microfluidics or fabrication of metasurfaces [1, 2]. In this work feasibility to fabricate large aspect ratio channels in soda-lime glass using direct laser ablation and wet chemical etching through thin chromium mask was investigated. The fabrication process consists of three steps: selective removal of chromium film, using laser, glass etching through apertures in chromium film, removal of chromium film (Figure 1).



Figure 1. Fabrication of large aspect ratio channels in soda-lime glass using direct laser ablation and wet chemical etching through thin chromium mask.

Using a picosecond laser, dimples were ablated in glass samples, coated with thin chromium film. They were etched in KOH solution for different time intervals and compared with non-etched samples. After the experiment, the samples were investigated using Sensofar optical profiler, where the channel depth and its entrance width data were obtained. Dependence of channel entrance width, depth and aspect ratio on laser fluence and number of pulses per spot were found (Figure 2).

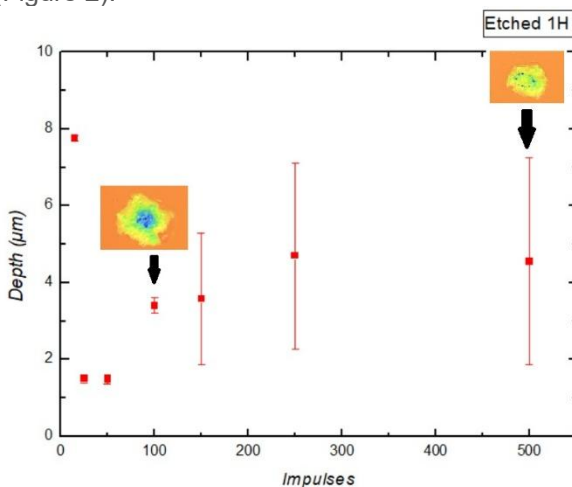


Figure 2. Dependence of channel depth on number of laser pulses per spot after 1 hour etching in 8M KOH water solution.

References

1. Patrice Genevet, Federico Capasso, Francesco Aieta, Mohammadreza Khorasaninejad, and Robert Devlin Recent advances in planar optics: from plasmonic to dielectric metasurfaces, *Optica*, 4(1), pp. 139-152 (2017).
2. Felix Sima and Koji Sugioka. "Ultrafast laser manufacturing of nanofluidic systems" *Nanophotonics*, (9), pp. 2389-2406, (2021).

TERAHERCINIŲ VAIZDŲ RAIŠKOS GERINIMAS NAUDOJANT NEURONINIUS TINKLUS

Ugnė Šilingaitė¹, Ignas Grigelionis¹

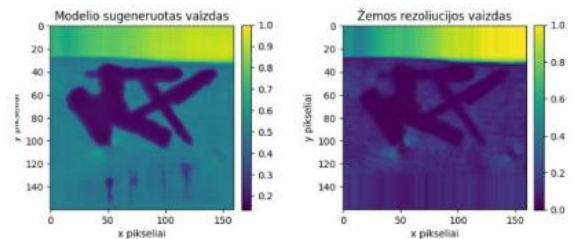
¹Fizinių ir Technologijos Mokslų Centras, Optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: ugne.silingaite@ftmc.lt

Terahercinė (THz) spinduliuotė (bangos ilgai tarp 0,3 mm iki 3 mm) yra intensyviai tiriama dėl savo plačių panaudojimo galimybių įvairiose srityse, įskaitant saugumo patikros punktus. Šio bangų ruožo elektromagnetinė spinduliuotė gali prasiskverbti pro plonus dielektrinių medžiagų sluoksnius, pavyzdžiui popierių, plastiką arba drabužius, tačiau nepraeina pro metalą, todėl ją galima naudoti paslėptiems objektams aptikti [1]. Deja, dėl ilgų vaizdinimo laikų ir jautrių jutiklių matricių trūkumo THz vaizdai dažnai nėra geros raiškos, o ją padidinti bandoma skaitmeniškai, pvz. naudojantis neuroniniais tinklais [2]. Šiame darbe THz vaizdų raiška yra gerinama naudojant DeblurGan [3] architektūros neuroninius tinklus, kurie yra pritaikyti gerinti objektus uždengtus tam tikra medžiaga (1 pav.), kuriai nustatyti yra naudojamas kitas, klasifikuojantis konvoliucinis neuroninis tinklas. Šiame darbe apmokytas klasifikacijos modelis pasiekė 83% tikslumą klasifikuodamas skirtingas medžiagas, o apmokyti 9 generatyvūs besivaržančių tinklų (GAN) modeliai, skirti gerinti skirtingomis medžiagomis uždengtų objektų skyrą, geba išryškinti objektus THz nuotraukoje sumažindami fono įtaką. Didžiausio signalo-triukšmo santykio skirtumo vertės mokymo duomenims yra intervale nuo 12,45 dB (medžio atveju) iki 22,44 dB (niekuo neuždengto objekto vaizdo skyros gerinimo atveju).

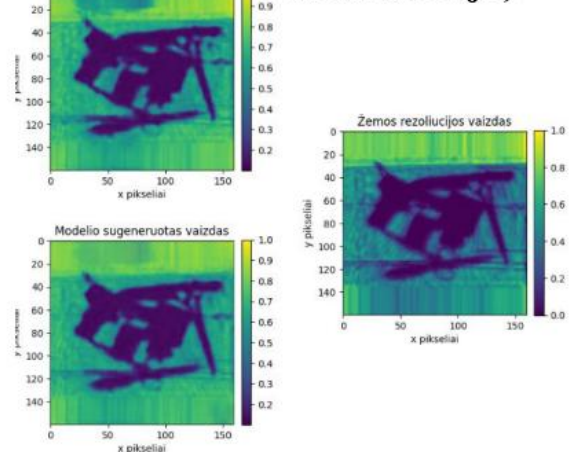
Literatūra:

1. SEO, M., PARK, H. „Terahertz Biochemical Molecule-Specific Sensors“. *Advanced Optical Materials* [interaktyvus]. 2019, 8(3), 1900662 [žiūr. 2025-01-13]. ISSN 2195-1071. Prieiga per: doi:10.1002/adom.201900662
2. LI, Yade, et al. „Adaptive terahertz image super-resolution with adjustable convolutional neural network“. *Optics Express* [interaktyvus]. 2020, 28(15), 22200 [žiūr. 2023-05-17]. Prieiga per: doi:10.1364/oe.394943.
3. KUPYN, O., et al. „DeblurGAN: Blind Motion Deblurring Using Conditional Adversarial Networks“. In: *2018 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)* [interaktyvus]. IEEE, 2018 [žiūr. 2023-05-17]. ISBN 9781538664209. Prieiga per: doi:10.1109/cvpr.2018.00854

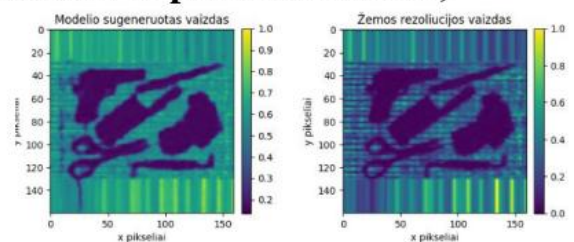
medis



putplastis (viršuje - klaidinga klasifikacija)



tinklelis ir polikarbonatas;



1 pav. Viršuje – teisingai suklasifikuotų THz vaizdų gerinimas su atitinkamu GAN modeliu, kur objektai uždengti medžiu. Viduryje - putplasčiu, klaidingai suklasifikuoto kaip grindų danga, uždengto vaizdo skyros gerinimas „neteisingu“ (modeliu skirtu gerinti grindų danga uždengtų objektų vaizdus) ir „teisingu“ (modeliu, skirtu gerinti putplasčiu uždengtų objektų vaizdus) GAN modeliais. Apačioje – vaizdo, uždengtų keliomis medžiagomis (tinkliu ir polikarbonatu) gerinimas.

Ar kosmologiniai modeliai atkuria stebimas galaktines t kmes?

Milda Valyt ¹, Kastytis Zubovas¹

¹Fizini  ir technologijos moksl  centras, Fundamentini  tyrim  skyrius
Saul tekio al. 3, LT-10257 Vilnius, el. p.: milda.valyte@ftmc.lt

Galaktik  centruose aptinkamos juodosios skyl s (BH) auga epizodiškai, vykstant intensyviai dujų akrecijai. Šie intensyvios akrecijos epizodai į BH yra vadinami aktyviu galaktikos branduoliu (AGN) [1]. Turimi AGN stebėjim  duomenys suteikia empirinę atramą kosmologini  modeli  vystymui, o pastarieji suteikia galimyb  analizuoti 3D dujų kinematiką bei evoliuciją, taip pat turime didesnes aktyvi  galaktik  imtis statistinei analizei. Tyrimai rodo, kad AGN varomos t km s reikšmingai veikia tarp vaig din  terp  bei reguliuoja  vaig d darą. Norint suprasti pagrindinius t kmi  varymo mechanizmus, yra b tina įvertinti, kaip pa ios galaktikos savyb s, tokios kaip  vaig d daros sparta (SFR), galaktikos  vaig din  mas  (M_ ) ir AGN šviesis (L_{AGN}) siejasi su pagrindin mis galaktini  t kmi  savyb mis. Šiame tyrime ypatingas dėmesys skiriamas t km s mas s pernašos spartos $\dot{M}$ analizei.

Darbe yra analizuojami didel s raiškos hidrodinaminio kosmologinio IllustrisTNG50 modelio duomenys, gauti naudojant judan ios gardel s kodą AREPO [2]. Modelyje aktyvios galaktikos bei jose besiformuojan ios t km s yra identifikuojamos keliais  ingsniais: pirmiausia, naudojantis TNG50 grupi  katalogais, kur atskiros dalel s jau yra suskirstytos į didesnius objektus pasitelkiant kaimynn  paieškos algoritmus, apribojama duomen  imtis bei nustatoma realistiška  vaig din s mas s riba galaktikoms, kuri  aktyvumas toliau analizuojamas [3]. Susiaurinus t kmi  paiešk  sritį toliau analizuojama sistemos momentinė nuotrauka bei t kmi  ieškoma įvertinant galaktikos kinematin s savyb s. Gauti modeliuojam  t kmi  ir galaktik  parametrai bei iŗvedamos daugiamat s regresijos lygtys, aprašan ios mas s pernašos spartos d sningumus, leid ia rezultatus palyginti su stebėjim  duomenimis [4].

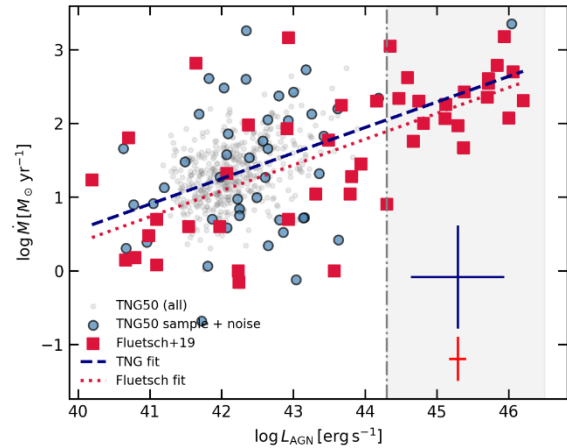
Markovo grandin s Monte-Karlo metodu nustatomos modeli  duomen  mas s pernašos spartos t km je priklausomyb s nuo pagrindini  galaktikos parametr  ( r. 1 lygtį):

$$\log\left(\frac{\dot{M}}{M_{\odot}\text{yr}^{-1}}\right) = 0,53 \log\left(6,63 \frac{\text{SFR}}{M_{\odot}\text{yr}^{-1}} + 0,10 \frac{L_{\text{AGN}}}{10^{43}\text{erg s}^{-1}}\right) - 0,02 \log\left(\frac{M_{\star}}{10^{11}M_{\odot}}\right) + 1,25 \quad (1)$$

Kadangi mas s pernašos spartos reik m  smarkiai priklauso nuo pasirinkto apskai iavimo metodo, papildomai tikrinama, ar stebim  priklausomybi  sklaidą galima atkurti prie modeli  duomen  prid jus sintetinį gausinį triukšmą. Rezultatai rodo, kad prid jus triukšmą sklaida abiejose a yse tampa panaši į stebėjim , ta iau stebimam d sningumui atkurti reikalingos paklaid  vert s yra didesn s nei cituojama stebėjim  darbuose [4].

Bendresni palyginimai rodo, kad TNG50 modelyje yra labai ma ai aukštu AGN šviesiu pasi ymin i  galaktik , atkuriamos t km s yra ma iau energingos ir

l tesn s. Taip pat, modelyje atkuriamas reik mi  intervalas yra siauresnis lyginant su stebėjimais, kai vertinami visi tiriami galaktikos parametrai: L_{AGN}, SFR ir M_ .



1 pav. Mas s pernašos spartos t km je priklausomyb  nuo AGN šviesio vietin s Visatos galaktikoms. M lyni taškai  ymi atsitiktinai atrinktas 45 modeliuojamas galaktikas, raudoni kvadratai – Fluetsch et al. (2019) darbe pristatyti 45 t kmi  matavimai, pilki taškai – visos TNG50 modelyje aptikt  aktyvi  galaktik  vert s. Vertikali punktyrin  linija  ymi TNG50 modeliu atkuriamo AGN šviesio ribą, o m lynas ir raudonas kry iai – paklaid  ribos, atitinkamai modeliuojamoms bei stebimoms galaktikoms.

Literat ra

1. Harrison, C. M., & Ramos Almeida, C. 2024, *Galaxies*, 12, 17
2. Nelson, D., Pillepich, A., Springel, V., et al. 2019, *MNRAS*, 490, 3234
3. Dolag, K., Borgani, S., Murante, G., & Springel, V. 2009, *MNRAS*, 399, 497
4. Fluetsch, A., Maiolino, R., Carniani, S., et al. 2019, *MNRAS*, 483, 4586

Fazės pokyčio priklausomybė nuo geometrijos formuojant daugiasluoksnes modifikacijas lydytame kvarce femtosekundiniu lazeriu

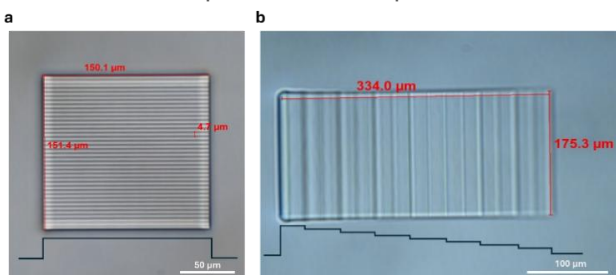
Eimantas Dermauskas¹, Valdemar Stankevič¹

¹ Fizinių ir technologijos mokslų centras, lazerinių technologijų skyrius
Savanorių pr. 231, LT-02300 Vilnius, el. p.: eimantas.dermauskas@ftmc.lt

Tūrinių fazinių elementų įrašymas skaidrioje terpėje yra svarbi šiuolaikinės fotonikos srities atšaka, kuri turi daug įvairių pritaikymų optinėje komunikacijoje arba kvantinėje fotonikoje [1]. Veikiant stipriai sufokusuota femtosekundinio lazerio spinduliuote lydytame kvarce galima suformuoti įvairaus tipo modifikacijas [2]. Šiame darbe daugiausia koncentruojamasi į I tipo modifikaciją [3], t.y. tūrinį lūžio rodiklio pokytį sufokusuotoje srityje. Formuojant šį pokytį itin svarbu išlaikyti lūžio rodiklio vientisumą ir užtikrinti proceso parametrų stabilumą. Todėl šiame darbe, pasitelkiant interferencinio matavimo metodiką, tiriamas tūryje suformuotas fazės pokytis, stabilumas ir jo priklausomybės nuo įrašymo parametrų.

Darbo tikslas – suformuoti tūrinę modifikaciją skirtinguose gyliuose lydytame kvarce, siekiant, kad dėl sferinių aberacijų modifikacijos ašinis ilgis pailgėtų ir būtų pasiektas kuo didesnis modifikacijos ilgis per vieną skenavimą [4]. Tokiu būdu, kombinuojant sluoksnius, galima valdyti bendrą fazės pokytį formuojant tūrio fazinius optinius elementus.

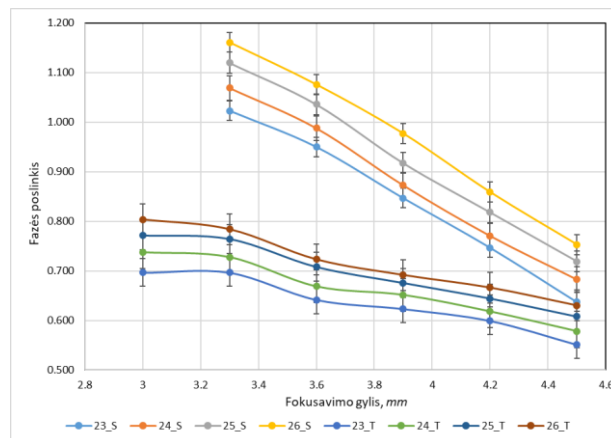
Eksperimento metu įrašomos stačiakampės ir trikampės daugiasluoksnės prizmės (pav. 1) bei tiriamas susidaręs fazės skirtumas stiklo tūryje, priklausomai nuo įrašymo parametrų. Tyrimui pasirinkta struktūras formuoti 515 nm bangos ilgio, 340 nJ energijos femtosekundinio lazerio spinduliuote, fokusavimo gyliuose nuo 3 iki 4,5 mm, kas 0,3 mm žingsniu. Įrašyta po 7 piramidines struktūras, turinčias 21–27 sluoksnius, ir po 4 stačiakampes struktūras, turinčias 23–26 sluoksnius. Sluoksnių persiklojimas (overlay) sudaro 42,5 %. Stačiakampės prizmės pagrindas yra 150 x 150 μm kvadratas, o trikampės prizmės stačiakampis – 335 x 175 μm.



Pav. 1 Stačiakampės (a) ir trikampės (piramidės) (b) prizmės, įrašytos stiklo tūryje, pagrindo matmenys ir skerspjūvis parodantis modifikacijos storio profilį atitinkantį fazės pokytį

Tiriama įrašytų struktūrų fazės poslinkio priklausomybė nuo gylio lydytame kvarce, sluoksnių skaičiaus bei struktūrų geometrijos. Rezultatų patikimumui, daryta 10 įrašymų su trikampėmis

prizmėmis ir 5 įrašymai su stačiakampėmis.



Pav. 2 Interferenciniu metodu išmatuoto stačiakampių ir trikampių prizmių fazės poslinkio priklausomybė nuo fokusavimo gylio. S- stačiakampė, T- trikampė prizmė.

Iš fazės poslinkio priklausomybės nuo gylio grafikų (pav. 2) matyti, kad didėjant įrašymo gyliui fazės poslinkis mažėja, kas siejama su spindulio sugertimi ir sferinėmis aberacijomis. Tačiau didinant sluoksnių skaičių šį sumažėjimą galima iš dalies kompensuoti. Lyginant stačiakampių ir trikampių prizmių fazės poslinkio grafikus, pastebimas reikšmingas skirtumas priklausomai nuo įrašymo gylio. Trikampėse prizmėse fazės poslinkis nė vienu atveju nepasiekia vertės, lygios 1, tuo tarpu stačiakampėse prizmėse 3 mm gylyje jau formuojasi nanogardelės.

Įrašant stačiakampes prizmes, modifikacijos yra žymiai stabilesnės, o bendrą fazės poslinkį galima lengviau valdyti nei trikampių prizmių geometrijoje. Dėl didesnio tūrinio užpildymo stačiakampės prizmės pasižymi didesniu fazės poslinkiu, palyginti su trikampėmis prizmėmis, įrašytomis tais pačiais parametrais.

Literatūra

1. Dezhi Tan, Zhuo Wang, Beibei Xu, Jianrong Qiu, Adv. Photon. 3, 024002 (2021).
2. C. Hnatovsky, J. R. Taylor, P. P. Rajeev, E. Simova, V. R. Bhardwaj, D. M. Rayner, and P. B. Corkum, Appl. Phys. Lett. **87**, 14104 (2005).
3. V. R. Bhardwaj, E. Simova, P. B. Corkum, D. M. Rayner, C. Hnatovsky, R. S. Taylor, B. Schreder, M. Kluge, J. Zimmer, J. Appl. Phys., **97** (8): 083102 (2005).
4. Stankevič V, Karosas J, Račiukaitis G, Gečys P, Opt Express **31**(3), 4482 (2023).

PLOKŠČIŲJŲ THZ OPTIKOS ELEMENTŲ PALYGINIMAS SKAITMENINIAME VAIZDINIMO EKSPERIMENTE

Paulius Kizevičius¹, Sergejus Orlovas¹

¹Fizinių ir technologijos mokslų centras, Optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: paulius.kizevicius@ftmc.lt

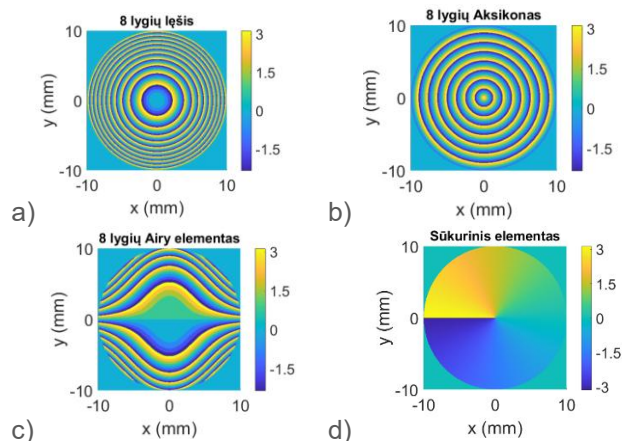
Lazerinėje pramonėje vis didesnę įtaką pluoštų formavimui įgauna fotoniniai plokščiosios optikos elementai. Šie elementai, skirtingai negu tradiciniai sferiniai lęšiai, yra plonesni, lengvesni, kompaktiškesni bei neįneša aberacijų į optinę sistemą. Tokie difrakciniai elementai pagerina objektų vaizdinimo raišką ir leidžia lanksčiai kontroliuoti elektromagnetinių bangų pluošto židinio struktūrą. Būtent pluošto struktūra židinio aplinkoje yra svarbus parametras, dėl kurio netradiciniai lazeriniai pluoštai pritaikomi plačiame elektromagnetinės spinduliuotės dažnių ruože – nuo optinio iki terahercų.

Viena iš svarbesnių specialiosios optikos taikymo sričių yra objektų vaizdinimas, jų atpažinimas, medžiagų detekcija ir bandinių inspekcija. Šios užduotys glaudžiai susijusios su difrakcijos teorija.

Dažniausiai iš lazerio išeinančios spinduliuotės kompleksinį elektrinio lauko skirstinį galime apibūdinti kaip Gauso pluoštą. Sklisdamas šis pluoštas difraguoja nuo pluošto sąsmaukos, o intensyvumas silpnėja. Tai yra viena iš priežasčių, kodėl praktikoje vis didesnę įtaką įgauna taip vadinami nedifraguojantys pluoštai. Vienas tokių yra Beselio pluoštas, kurio skersinio intensyvumo skirstinys nepriklauso nuo atstumo z ir nediverguoja [1]. Kitas yra Airy pluoštas, kuris taip pat išsaugo savo formą, tačiau centrinis maksimumas yra paslinktas ir sklinda išlenkta paraboline trajektorija [2].

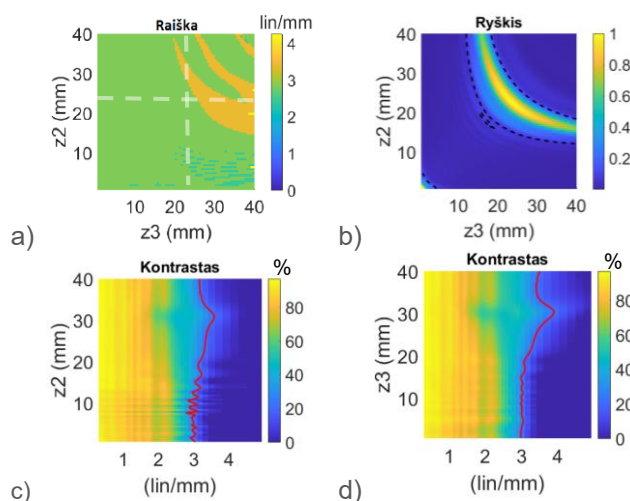
Šie pluoštai paprastai generuojami erdviniais šviesos modulatoriais arba plokščiaisiais fotoniniais difrakciniais elementais, kurie šviesos pluošto frontui priskiria tam tikrą fazinę ir (arba) amplitudinę moduliaciją. Tokios šviesos panaudojimas ir optimalus optinių elementų išdėstymas gali lemti dar aukštesnę vaizdo raišką, ryškumą ir kontrastą, o tai yra vienas pagrindinių vaizdavimo teorijos tikslų [3].

Šiame darbe bus pristatyti sumodeliuoti faziniai difrakciniai elementai ir jų generuojami pluoštai, skirti veikti 0,6 THz ($\lambda = 0,5$ mm) spinduliuotei. Taip pat bus pateikta virtualaus vaizdinimo rezultatų analizė kiekvieno elemento atveju.



pav. 1. Sumodeliuoti faziniai elementai.

Šio darbo idėja – vaizdinimo eksperimente panaudoti ir struktūrinę šviesą. Buvo siekiama išanalizuoti ne tik klasikinio Gauso pluošto THz vaizdinimą, bet ir specialiosios optikos elementų taikymo galimybes. Siekiant palyginti gautų vaizdų kokybę, vertinti raiškos, ryškio ir kontrasto žemėlapiai, taip pat nagrinėta, ar įmanoma pasiekti aukštos kokybės vaizdą didesnėje objekto ir atvaizdo skirtyje, t. y. ar galima pagerinti lauko bei fokusavimo gylį.



pav. 2. Gauso-Gauso vaizdinimo atvejo raiškos a) ir ryškio b) priklausomybė nuo surenkančiojo lęšio (z_2) ir detektoriaus pozicijos (z_3). c) ir d) kontrasto priklausomybė nuo atstumų z_2 ir z_3 ties didžiausio ryškio pozicija. Juoda punktyrinė linija žymi 10% ryškio lygį, raudonas kontūras žymi 20% kontrasto vertės ribą.

Literatūra

1. D. McGloin, K. Dholakia, Bessel beams: diffraction in a new light, Contemporary Physics 46(1), 15–28 (2005).
2. G. A. Siviloglou, D. N. Christodoulides, Accelerating finite energy airy beams, Optics letters 32(8), 979–981 (2007).
3. S. Orlov, R. Ivaškevičiūtė-Povilauskienė, and P. Kizevičius et al., “Light engineering and silicon diffractive optics assisted nonparaxial terahertz imaging,” Laser Photonics Rev. 18, 2301197 (2024).

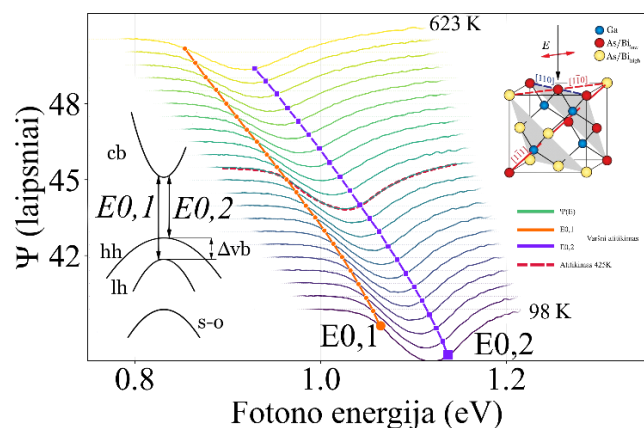
Bismuto koncentracijos įtaka GaAs_{1-x}Bi_x optinėms savybėms

A. Mikalauskas¹, S. Tumėnas¹

¹Fizinių ir technologijos mokslų centras, optoelektronikos skyrius
Saulėtekio al. 3, LT-10257 Vilnius, el. p.: aidas.mikalauskas@ftmc.lt

Bismuto įterpimas į GaAs sukuria praskiestus bismidinčius lydinius su milžinišku juostos siaurėjimu (~88 meV/%Bi) ir silpna temperatūrine priklausomybe, todėl jie tinka artimosios IR optoelektronikai. Dėl didelio Bi–As atomų dydžių skirtumo epitaksinio augimo metu savaime formuojasi CuPt_B tvarka, keičianti elektronines ir optines savybes^[1]. Nors MBE ant GaAs(001) užaugintuose GaAs_{1-x}Bi_x sluoksniuose CuPt_B patvirtinta, jos optinės savybės dar menkai ištirtos. Čia pateikiame elipsometrinį GaAs_{1-x}Bi_x (x=0,022–0,056) tyrimą, akcentuojant tvarkos sukeltą anomalią optinę anizotropiją.

Bandiniai: MBE užauginti ~500 nm GaAs_{1-x}Bi_x sluoksniai ant GaAs padėklų. HRXRD ir STEM patvirtino CuPt_B su B⁺ ir B⁻ povariantais [111] ir [111] kryptimis^[2]. Matavimai: kintamo kampo spektroskopinė elipsometrija 0,7–6 eV ir normalaus kritimo pralaidumo Miulero matricos elipsometrija 0,7–1,5 eV, 98–623 K temperatūroje



1 pav. GaAs_{0.944}Bi_{0.056} bandinio $\Psi(E)$ priklausomybė nuo temperatūros. Iš spektrų nustatytos kritinių taškų $E_{0,1}$ ir $E_{0,2}$ energijos bei jų poslinkis. Įterpinys kairėje parodo CuPt tvarkos sukeltą valentinės juostos skilimą Δ_{vb} , o įterpinys dešinėje – CuPt_B tipo tvarkos GaAs_{1-x}Bi_x gardelėje schemą^[3]

Dielektrinės funkcijos tenzorius, nustatytas iš elipsometrijos duomenų, skiriasi vertės pagrindinėmis kristalografinėmis kryptimis. Esant B+/B- susitvarkymui dielektrinės funkcijos komponentės yra $\epsilon_{[110]} = (\epsilon_{\perp} + 2\epsilon_{\parallel})/3$, $\epsilon_{[110]} = \epsilon_{\perp}$ ir $\epsilon_{[001]} = (2\epsilon_{\perp} + \epsilon_{\parallel})/3$, kur $\epsilon_{\perp}$ ir $\epsilon_{\parallel}$ atitinka statmenas ir lygiagrečias komponentes tvarkos krypties atžvilgiu. Tai galima išreikšti kaip izotropinę dielektrinę funkciją su perturbacija $\epsilon_{[110]} = \epsilon(\omega) + \delta_{\perp}(\omega)$ ir $\epsilon_{[110]} = \epsilon(\omega) - \delta_{\perp}(\omega)$, o $\epsilon_{[001]} = \epsilon(\omega)$. Anizotropijos parametras $\delta_{\perp}(\omega)$ kiekybiškai apibūdina atominės tvarkos sukeltą optinės anizotropijos laipsnį. Miulero matricos elementų analizė atskleidė charakteringas spektroskopines ypatybes, susijusias su skilusios valentinės juostos perėjimais.

Fundamentalus sugerties kraštas skyla į du atskirus perėjimus $E_{0,1} = 1,008$ eV ir $E_{0,2} = 1,008$ eV bandiniuose su $x = 0,056$, atskirtus maždaug 80 meV tarpu. Optinės anizotropijos dydis, apibūdinamas $\delta_{\perp}(\omega)$ maksimumo vertėmis, rodo ryškius maksimumus ties šiomis perėjimų energijomis ir sistemingai didėja su bismuto koncentracija, tiesiogiai koreliuodamas su atominės tvarkos laipsniu.

Temperatūriniai elipsometrinio ψ parametro matavimai pralaidumo režime parodė tvarkos sukeltos optinės anizotropijos terminį stabilumą. Nors abu skilę perėjimai $E_{0,1}$ ir $E_{0,2}$ demonstruoja laukiamą raudonąjį poslinkį didėjant temperatūrai (98 K–623 K), sekdami tipinę puslaidininkių draustinės juostos temperatūrinę priklausomybę, energijos skirtumas $\Delta_{VB} = E_{0,2} - E_{0,1}$ išlieka pastovus, apie 80 meV visame temperatūrų diapazone. Ši skilimo dydžio nepriklausomybė nuo temperatūros patvirtina jo struktūrinę kilmę iš atominės tvarkos, o ne įtempimų efektų, kurie rodytų reikšmingą temperatūrinį kitimą dėl diferencinio terminio plėtimosi. Valentinės juostos skilimas, stebimas elipsometrijos metodais, gali būti suprantamas kaip kylantis iš kombinuoto epitaksinio įtempimų ir atominės tvarkos poveikio. Bendras skilimas $\Delta_{VB} = \sqrt{(\Delta_c^2 + \Delta_e^2)}$ apima ir tvarkos sukeltos komponentės Δ_c , tiek įtempimų komponentės Δ_e indėlius. Bandinių su skirtingu tvarkos laipsniu analizė atskleidė, kad tvarkos indėlis didėja tiesiškai su bismuto koncentracija ir tvarkos parametru R, pasiekdamas 76 meV vertes esant $x = 0,056$ ir $R = 0,58$. Įtempimų indėlis kinta nuo 0 iki 29 meV priklausomai nuo gardelės nesutapimo ir relaksacijos būsenos.

Išsamūs elipsometriniai tyrimai nustatė, kad CuPt_B tipo tvarka pasižymintys GaAs_{1-x}Bi_x epitaksiniai sluoksniai demonstruoja ryškią optinę anizotropiją. Fundamentalaus optinio perėjimo skilimas į dvi komponentes, atskirtas 40–100 meV tarpu priklausomai nuo bismuto koncentracijos, sukuria galimybes poliarizacijai jautriems prietaisų taikymams. Šių efektų terminis stabilumas iki 623 K, patvirtintas temperatūrine elipsometrija, demonstruoja CuPt tipo tvarka pasižyminčių bismidų tinkamumą praktiniams optoelektroniniams taikymams, reikalaujantiems veikimo aukštose temperatūrose.

Literatūra

1. Paulauskas T., Čechavičius B. et al. Journal of Applied Physics, 2020, t. 128, p. 195106
2. Paulauskas T., Tumėnas S. et al. Scientific Reports, 2022, t. 12, p. 7707.
3. Karpus V., Čechavičius B. et al. Journal of Physics D: Applied Physics, 2021, t. 54, p. 504001.

P50 did not attend.

Humidity-Induced Stress Variations in Nanostructured GLAD Coatings for High-LIDT Optical Mirrors

Adomas Strazdas¹, Simas Melnikas¹, Lukas Ramalis¹

¹Center for Physical Sciences and Technology, Department of Laser Technologies
Saulėtekio av. 3, LT-10257 Vilnius, email: Adomas.strazdas@ftmc.lt

Optical components are essential in laser systems used to direct and control laser-generated radiation. Demands for optical elements, including mirrors, are rapidly increasing, therefore making such elements a weakest link when it comes to laser-induced damage threshold (LIDT). To gain benefits in optical resistivity or spectral performance, a fairly new method is developed using nanostructured thin films coated by GLancing Angle Deposition (GLAD) method. Conventional Titanium oxide mirrors with low LIDT can be enhanced by depositing an additional “upgrade” [1] coating to improve LIDT. These “upgrade” layers are highly porous and may absorb water from the environment. In order to solve this issue, environmental stability measurements are investigated.

The aim of this study is to investigate the dependence of nanostructured coating stress on humidity. The upgrade 5 layer coating consists of 2 porous silica layers with low refractive index deposited at substrate tilt angle of 70° and 3 dense hafnia (deposited at 0°) with high refractive index. Porous films tend to absorb water and can induce some instabilities depending on humidity in the environment. Water molecule movement changes the intrinsic stress values of the film a considerable amount, and may lead to coating cracking.

To test this hypothesis, a gas chamber was built around an interferometer to measure the stress of porous coatings under different humidities. At first you insert the porous film, measure the peak-to-valley values, and start introducing nitrogen gas, to lower the humidity. During this test measurements are made every 5rh% drop in humidity and after reaching 7,5rh% every 10 minutes, and later out of the chamber humidity. To get higher humidity a container with a water salt mixture [2] was place inside to create a more humid atmosphere, and the measurements would be similar to low humidity. The measurements took turns at several different levels of humidity, and after some time in both highest and lowest achieved humidity, which was about 5 %rh and 79 %rh.

The obtained results demonstrate that as we decrease the humidity the stress increases, as we can see from the graphs below. The peak-to-valley values changed from 0.625 λ to 1.202 λ (figure 1), as humidity was lowered to 5RH%. This change indicates that by having a higher humidity, the power value may go down, and if the humidity is changed aggressively, we could crack the film from change in intrinsic stress.

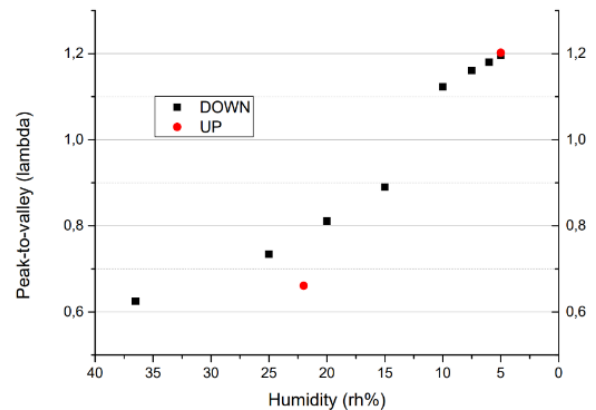


Figure 1. Dependence of peak-to-valley values of humidity as humidity decreases (DOWN) and recovers (UP).

All in all, we coated GLAD coatings on titanium/silicon mirrors which had low intrinsic stress. Afterwards it was discovered that the stress was dependent on humidity, and a lot of problems arose. If these issues were dealt with, such developed coatings could be of major use as they are aimed to be applied in ultrafast laser systems.

References

1. Grinevičiūtė L. et al., Appl. Surf. Sci. 541, 148599 (2021)
2. Greenspan L., J. Res. Natl. Bur. Stand. A Phys. Chem. 81A, 89-96 (1977)